* * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:51:01 ON 17 FEB 2005

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 14:51:13 ON 17 FEB 2005

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 15 FEB 2005 HIGHEST RN 831913-30-5
DICTIONARY FILE UPDATES: 15 FEB 2005 HIGHEST RN 831913-30-5

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\10751622e.str

chain nodes :
6 7 8 9 10 11
ring nodes :
1 2 3 4 5
chain bonds :
1-7 3-8 4-9 5-6 9-10 10-11
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-7 2-3 3-4 3-8 4-5 5-6 10-11
exact bonds :
4-9 9-10

G1:C,H,F,X,Cy,Ak

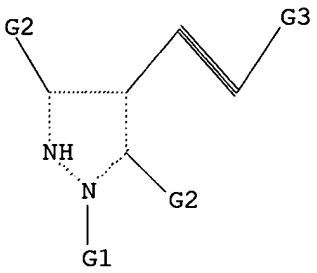
G2:C,H,Cl,F,CN,CHO,X,Cy,Ak,OH,NH,NH2,NH3,NO2,M

G3:Cy,Hy

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:Atom

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



G1 C,H,F,X,Cy,Ak

G2 C,H,Cl,F,CN,CHO,X,Cy,Ak,OH,NH,NH2,NH3,NO2,M

G3 Cy,Hy

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 14:51:32 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 67 TO ITERATE

100.0% PROCESSED 67 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 849 TO 1831
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 14:51:36 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1370 TO ITERATE

100.0% PROCESSED 1370 ITERATIONS 5 ANSWERS
SEARCH TIME: 00.00.01

L3 5 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 161.33 161.54

FILE 'CAPLUS' ENTERED AT 14:51:40 ON 17 FEB 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 17 Feb 2005 VOL 142 ISS 8
FILE LAST UPDATED: 16 Feb 2005 (20050216/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3/p
L4 1 L3/P

=> d ibib abs hitstr tot

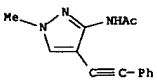
L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:781600 CAPLUS
DOCUMENT NUMBER: 132:237020
TITLE: Peculiarities of copper(I)- and palladium-catalyzed cross-coupling of terminal alkynes with vicinal amino- and (N-acetylamino)iodopyrazoles. Synthesis of alkynylaminopyrazoles
AUTHOR(S): Tretyakov, Eugene V.; Knight, David W.; Vasilevsky, Sergei F.
CORPORATE SOURCE: Institute of Chemical Kinetics and Combustion, Siberian Branch of the Russian Academy of Sciences, Novosibirsk, 630090, Russia
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1999), (24), 3713-3720
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:237020

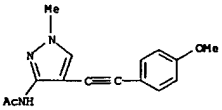
AB A number of vicinal amino- and (N-acetylamino)alkylpyrazoles have been synthesized by cross-coupling reactions of iodopyrazoles with alk-1-ynes using a combination of Pd(PPh3)2Cl2 and CuI as catalyst in Et3N or with copper acetylides. The latter Stephens-Castro reaction of copper acetylides with these amino- and (N-acetylamino)iodopyrazoles was established as a common method for the preparation of (N-acetylamino)alkynylpyrazoles. The Pd/Cu-catalyzed cross-coupling of iodopyrazoles (Sonogashira reaction) with alk-1-ynes bearing electron-releasing substituents was unsuitable for the synthesis of alkynylpyrazoles: 3- and 5-iodopyrazoles were unreactive but, in the case of 4-iodo derivs., reductive deiodination, accompanied by homocoupling of the alk-1-yne component, was the only reaction.

IT **260442-56-6P 260442-58-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(copper(I)- and palladium-catalyzed cross-coupling of terminal alkynes with vicinal amino- and (N-acetylamino)iodopyrazoles)

RN 260442-56-6 CAPLUS
CN Acetamide, N-[1-methyl-4-(phenylethynyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

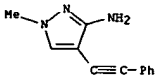


RN 260442-58-8 CAPLUS
CN Acetamide, N-[4-[(4-methoxyphenyl)ethynyl]-1-methyl-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

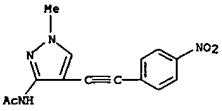


IT **220637-81-0P 260442-50-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(copper(I)- and palladium-catalyzed cross-coupling of terminal alkynes with vicinal amino- and (N-acetylamino)iodopyrazoles)

RN 220637-81-0 CAPLUS
CN 1H-Pyrazol-3-amine, 1-methyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)



RN 260442-50-0 CAPLUS
CN Acetamide, N-[1-methyl-4-[(4-nitrophenyl)ethynyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

* * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:54:36 ON 17 FEB 2005

=> file reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 14:54:45 ON 17 FEB 2005

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 15 FEB 2005 HIGHEST RN 831913-30-5
DICTIONARY FILE UPDATES: 15 FEB 2005 HIGHEST RN 831913-30-5

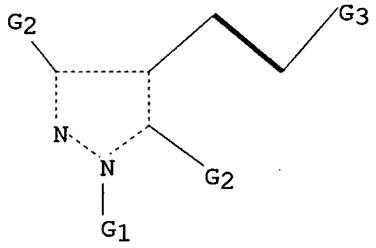
TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

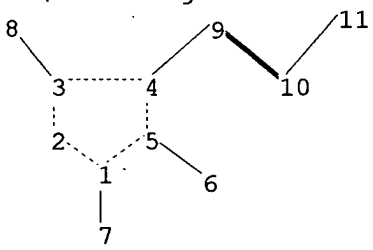
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\10751622g.str





chain nodes :
6 7 8 9 10 11
ring nodes :
1 2 3 4 5
chain bonds :
1-7 3-8 4-9 5-6 9-10 10-11
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-7 2-3 3-4 3-8 4-5 5-6 10-11
exact bonds :
4-9 9-10

G1:C,H,F,X,Cy,Ak

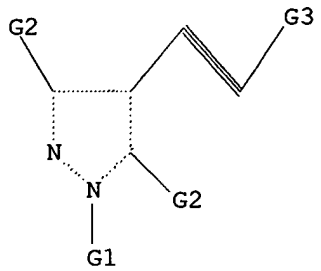
G2:C,H,Cl,F,CN,CHO,X,Cy,Ak,OH,NH,NH2,NH3,NO2,M

G3:Cy,Hy

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:Atom

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



G1 C,H,F,X,Cy,Ak

G2 C,H,Cl,F,CN,CHO,X,Cy,Ak,OH,NH,NH2,NH3,NO2,M

G3 Cy,Hy

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 14:55:06 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 67 TO ITERATE

100.0% PROCESSED 67 ITERATIONS 5 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 849 TO 1831
PROJECTED ANSWERS: 5 TO 234

L2 5 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 14:55:10 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1370 TO ITERATE

100.0% PROCESSED 1370 ITERATIONS 164 ANSWERS
SEARCH TIME: 00.00.01

L3 164 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 161.33 161.54

FILE 'CAPLUS' ENTERED AT 14:55:14 ON 17 FEB 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 17 Feb 2005 VOL 142 ISS 8
FILE LAST UPDATED: 16 Feb 2005 (20050216/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3/p
L4 48 L3/P

=> d ibib abs hitstr tot
THE ESTIMATED COST FOR THIS REQUEST IS 237.12 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L4 ANSWER 1 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:1156446 CAPLUS
DOCUMENT NUMBER: 142:74603
TITLE: Preparation of thienopyrimidines as inhibitors of ErbB kinases
INVENTOR(S): Badiang, Jennifer G.; Dickerson, Scott Howard; Donaldson, Kelly Horne; Hinkle, Kevin Wayne; Hornberger, Keith Robert; Petrov, Kimberly Glennon; Reno, Michael John; Stevens, Kirk Lawrence; Uehling, David Edward; Waterson, Alex Gregory
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 103 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004112714	A2	20041229	WO 2004-US19388	20040617

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2003-479567P P 20030618
GI

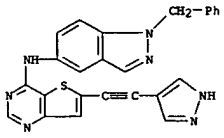
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [one of A1 and A2 = S, CH; R1 = heteroaryl, heteroarylene, arylene; R2 = H, alkyl; R3 = arylene, heteroarylene] are prepared For instance, N-[3-Chloro-4-[(3-fluorobenzyl)oxy]phenyl]-6-((pyridin-2-yl)ethynyl)thieno[2,3-d]pyrimidin-4-amine is prepared from 6-bromo-N-[3-chloro-4-[(3-fluorobenzyl)oxy]phenyl]thieno[2,3-d]pyrimidin-4-amine and 2-iodopyridine. Compds. of the invention have pIC50 of 5.5 or greater for EGFR kinase, ErbB-2 kinase and ErbB-4 kinase. I are useful for the treatment of diseases associated with inappropriate ErbB family kinase activity.

IT **815609-72-4P 815609-73-5P 815609-74-6P 815609-75-7P 815609-76-8P 815609-77-9P 815609-78-0P 815609-79-1P 815609-80-4P 815609-81-5P 815609-82-6P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of thienopyrimidines as inhibitors of ErbB kinases)

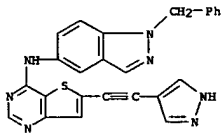
RN 815609-72-4 CAPLUS
CN Thieno[2,3-d]pyrimidin-4-amine, N-[3-chloro-4-[(3-fluorophenyl)methoxy]phenyl]-6-(1H-pyrazol-4-ylethynyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

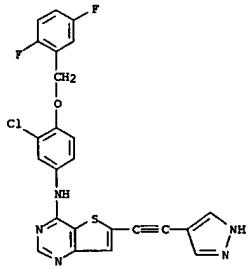


● HCl

RN 815609-75-7 CAPLUS
CN Thieno[3,2-d]pyrimidin-4-amine, N-[1-(phenylmethyl)-1H-indazol-5-yl]-6-(1H-pyrazol-4-ylethynyl)- (9CI) (CA INDEX NAME)

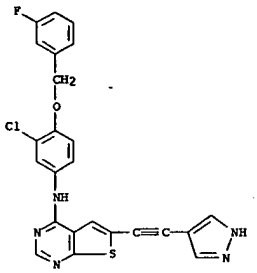


RN 815609-76-8 CAPLUS
CN Thieno[3,2-d]pyrimidin-4-amine, N-[3-chloro-4-[(2,5-difluorophenyl)methoxy]phenyl]-6-(1H-pyrazol-4-ylethynyl)- (9CI) (CA INDEX NAME)

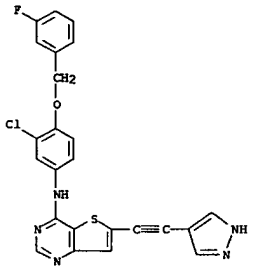


RN 815609-77-9 CAPLUS

L4 ANSWER 1 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



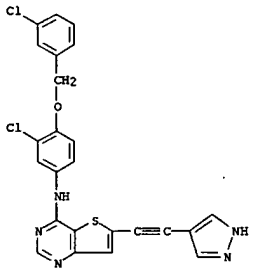
RN 815609-73-5 CAPLUS
CN Thieno[3,2-d]pyrimidin-4-amine, N-[3-chloro-4-[(3-fluorophenyl)methoxy]phenyl]-6-(1H-pyrazol-4-ylethynyl)- (9CI) (CA INDEX NAME)



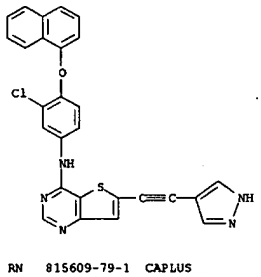
RN 815609-74-6 CAPLUS
CN Thieno[3,2-d]pyrimidin-4-amine, N-[1-(phenylmethyl)-1H-indazol-5-yl]-6-(1H-pyrazol-4-ylethynyl)-, monohydrochloride (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

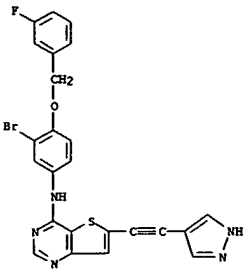
CN Thieno[3,2-d]pyrimidin-4-amine, N-[3-chloro-4-[(3-chlorophenyl)methoxy]phenyl]-6-(1H-pyrazol-4-ylethynyl)- (9CI) (CA INDEX NAME)



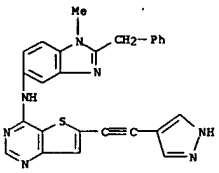
RN 815609-78-0 CAPLUS
CN Thieno[3,2-d]pyrimidin-4-amine, N-[3-chloro-4-(1-naphthalenyloxy)phenyl]-6-(1H-pyrazol-4-ylethynyl)- (9CI) (CA INDEX NAME)



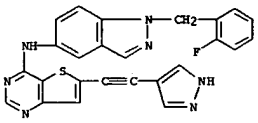
RN 815609-79-1 CAPLUS
CN Thieno[3,2-d]pyrimidin-4-amine, N-[3-bromo-4-[(3-fluorophenyl)methoxy]phenyl]-6-(1H-pyrazol-4-ylethynyl)- (9CI) (CA INDEX NAME)



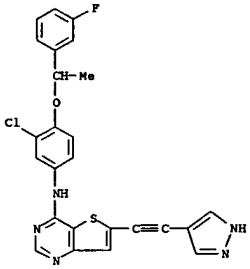
RN 815609-80-4 CAPLUS
CN Thieno[3,2-d]pyrimidin-4-amine, N-[1-methyl-2-(phenylmethyl)-1H-benzimidazol-5-yl]-6-(1H-pyrazol-4-ylethynyl)- (9CI) (CA INDEX NAME)



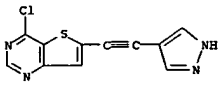
RN 815609-81-5 CAPLUS
CN Thieno[3,2-d]pyrimidin-4-amine, N-[1-[(2-fluorophenyl)methyl]-1H-indazol-5-yl]-6-(1H-pyrazol-4-ylethynyl)- (9CI) (CA INDEX NAME)



RN 815609-82-6 CAPLUS
CN Thieno[3,2-d]pyrimidin-4-amine, N-[3-chloro-4-[1-(3-fluorophenyl)ethoxy]phenyl]-6-(1H-pyrazol-4-ylethynyl)- (9CI) (CA INDEX NAME)



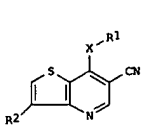
IT 815610-13-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of thienopyrimidines as inhibitors of ErbB kinases)
RN 815610-13-0 CAPLUS
CN Thieno[3,2-d]pyrimidine, 4-chloro-6-(1H-pyrazol-4-ylethynyl)- (9CI) (CA INDEX NAME)



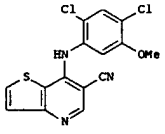
ACCESSION NUMBER: 2004:1036761 CAPLUS
DOCUMENT NUMBER: 142:6510
TITLE: Preparation of thieno[3,2-b]pyridine-6-carbonitriles as protein tyrosine kinase inhibitors
INVENTOR(S): Boschelli, Diane Harris; Zhang, Nan; Barrios, Sosa Ana Carolina; Durutlic, Haris; Wu, Biqi
PATENT ASSIGNEE(S): Wyeth, John, and Brother Ltd., USA
SOURCE: U.S. Pat. Appl. Publ., 75 pp., Cont.-in-part of U.S. Ser. No. 719,359.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004242883	A1	20041202	US 2004-845710	20040514
US 2004138251	A1	20040715	US 2003-719359	20031121
PRIORITY APPLN. INFO.:			US 2002-428862P P	20021125.
			US 2003-719359 A2	20031121

GI



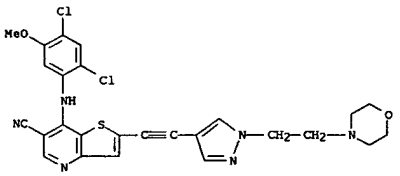
I



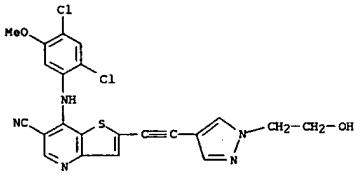
II

AB Title compds. I [wherein X = NH and derivs., O, SOm, NHCH2; m = 0-2; R1 = (un)substituted Ph; R2 = CHO, halo, R3, COXR3; R3 = (un)substituted alkyl, alkenyl, alkynyl, heteroaryl; and pharmaceutically acceptable salts thereof] were prepared as protein tyrosine kinase inhibitors. Four biol. assays are given. For example, II was prepared by amination of 7-chlorothieno[3,2-b]pyridine-6-carbonitrile (preparation given) with 2,4-dichloro-5-methoxyaniline in THF in the presence of NaH at reflux. Selected I displayed IC50 values in the range of 5.3 nM to 5040 nM for the inhibition of human recombinant Src kinase. Thus, I and their pharmaceutical compns. are useful in the treatment of neoplasm, stroke, osteoporosis, polycystic kidney disease, autoimmune disease, rheumatoid arthritis, and transplant rejection (no data).
IT 700845-03-0P, 7-[(2,4-Dichloro-5-methoxyphenyl)amino]-2-[[1-[2-(morpholin-4-yl)ethyl]-1H-pyrazol-4-yl]ethynyl]thieno[3,2-b]pyridine-6-carbonitrile 700845-69-8P, 7-[(2,4-Dichloro-5-methoxyphenyl)amino]-2-[[1-(2-hydroxyethyl)-1H-pyrazol-4-yl]ethynyl]thieno[3,2-b]pyridine-6-carbonitrile
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of thieno[3,2-b]pyridine carbonitriles as Src
kinase inhibitors for treatment of cancer, autoimmune disease, and related conditions)

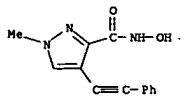
RN 700845-03-0 CAPLUS
CN Thieno[3,2-b]pyridine-6-carbonitrile, 7-[(2,4-dichloro-5-methoxyphenyl)amino]-2-[[1-[2-(4-morpholinyl)ethyl]-1H-pyrazol-4-yl]ethynyl]- (9CI) (CA INDEX NAME)



RN 700845-69-8 CAPLUS
CN Thieno[3,2-b]pyridine-6-carbonitrile, 7-[(2,4-dichloro-5-methoxyphenyl)amino]-2-[[1-(2-hydroxyethyl)-1H-pyrazol-4-yl]ethynyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 3 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:968067 CAPLUS
DOCUMENT NUMBER: 142:113958
TITLE: A new route to pyrazolo[3,4-c]- and -[4,3-c]pyridinones via heterocyclization of vic-substituted hydroxamic acids of acetylenylpyrazoles
AUTHOR(S): Mshvidobadze, Elena V.; Vasilevsky, Sergei F.; Elguero, Jose
CORPORATE SOURCE: Institute of Chemical Kinetics and Combustion, Siberian Branch of the Russian Academy of Sciences, Novosibirsk, 630090, Russia
SOURCE: Tetrahedron (2004), 60(51), 11875-11878
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The synthesis of 6-substituted pyrazolo[4,3-c]pyridin-4-ones, 6-substituted 5-hydroxypyrazolo[4,3-c]pyridin-6-ones, 5-substituted pyrazolo[3,4-c]pyridin-7-ones and 5-substituted 6-hydroxypyrazolo[3,4-c]pyridin-7-ones by heterocyclization of vic-acetylenylpyrazolehydroxamic acids under the influence of copper(I) salt in DMF or with organic bases in butanol or methanol is reported.
IT 823220-98-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrazolo[3,4-c]- and -[4,3-c]pyridinones via heterocyclization of vic-substituted hydroxamic acids of acetylenylpyrazoles)
RN 823220-98-0 CAPLUS
CN 1H-Pyrazole-3-carboxamide, N-hydroxy-1-methyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)

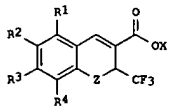


REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

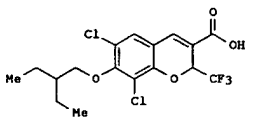
L4 ANSWER 4 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:857585 CAPLUS
DOCUMENT NUMBER: 141:350038
TITLE: Preparation of 2H-chromene-3-carboxylates and analogs as selective COX-2 inhibitors for treating inflammatory conditions
INVENTOR(S): Aston, Karl W.; Brown, David L.; Carter, Jeffrey S.; Deprow, Angela M.; Fletcher, Theresa R.; Hallinan, E. Ann; Hamper, Bruce C.; Huff, Renee M.; Kiefer, James R., Jr.; Koszyk, Francis; Kramer, Steven W.; Liao, Subo; Limburg, David; Springer, John R.; Tsymbalov, Sofya; Wang, Lijuan Jane; Xing, Li; Yu, Yi
PATENT ASSIGNEE(S): Pharmacia Corporation, USA
SOURCE: PCT Int. Appl., 799 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004087687	A1	20041014	WO 2004-IB939	20040319
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
NL 1025844	A1	20041001	NL 2004-1025844	20040329
PRIORITY APPLN. INFO.:			US 2003-459214P	P 20030331
OTHER SOURCE(S):	MARPAT 141:350038			

GI



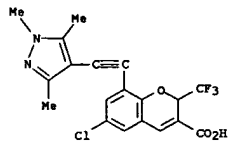
I



II

L4 ANSWER 4 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

AB Title benzopyrans I [wherein X = H, alkyl, pharmaceutically acceptable cation; Z = O, S, NH; R1-R4 = independently H, halo, OH, (un)substituted alkyl, alkenyl, alkynyl, alkoxy, amino, (hetero)aryl(oxy), etc.; and pharmaceutically acceptable salts thereof] were prepared via solution phase and solid phase parallel synthetic methods as cyclooxygenase-2 (COX-2) inhibitors. For example, cyclization of 2,4-dihydroxybenzaldehyde with Et 4,4,4-trifluorocrotonate gave Et 7-hydroxy-2-(trifluoromethyl)-2H-chromene-3-carboxylate (31.6%), which was etherified with 2-ethyl-1-butanol to afford the ethylbutoxy derivative (92%). Chlorination with Cl2 gas in the presence of Zn powder (49%), followed by saponification with NaOH (28.4%) provided II. The latter preferentially inhibited the production of prostaglandins by recombinant hCOX-2 over hCOX-1 with IC50 values of 0.0176 μM and 5.56 μM, resp. Thus, I and their pharmaceutical compns. are useful for the treatment of conditions associated with COX-2, such as inflammation.
IT 776321-09-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(COX-2 inhibitor; preparation of 2H-chromene-3-carboxylates and analogs as selective COX-2 inhibitors for treating inflammatory conditions)
RN 776321-09-6 CAPLUS
CN 2H-1-Benzopyran-3-carboxylic acid, 6-chloro-2-(trifluoromethyl)-8-[(1,3,5-trimethyl-1H-pyrazol-4-yl)ethynyl]- (9CI) (CA INDEX NAME)

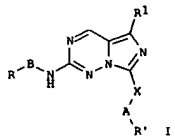


REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

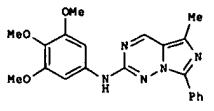
L4 ANSWER 5 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:857556 CAPLUS
DOCUMENT NUMBER: 141:350203
TITLE: Preparation of imidazotriazines as Polo-like kinases inhibitors for treatment of cancers
INVENTOR(S): Cheung, Mui; King, Nigel Paul; Kuntz, Kevin Wayne; Mook, Robert Anthony, Jr.; Pobanz, Mark Andrew; Salovich, James Michael; Wilson, Brian John
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 208 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004087652	A2	20041014	WO 2004-US9553	20040329
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRIORITY APPLN. INFO.:			US 2003-459293P	P 20030401
OTHER SOURCE(S):	MARPAT 141:350203			

GI



I



II

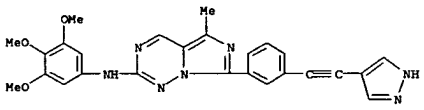
L4 ANSWER 5 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

AB Title compds. represented by the formula I [wherein R1 = alkyl; X = (CHR11)w; w = 0-1; R11 = H, alkyl; A, B= independently cycloalk(en)yl, aryl, 5-13 membered heterocyclyl and heteroaryl; R = [(R4)j-(R2)h-(Y2)g-(R2)f]n-; R' = -[(R2)a-(Y1)b-(R2)c-(R3)d]m; a,b,c,f,g,h = independently 0-1; d, j = independently 1-2; each R2 = independently alk(en/yn)ylene; Y1, Y2 = independently O, S(O)q, NH and derivs.; q = 0-2; each R3, R4 = independently H, halo, alk(en/yn)yl, cycloalk(en)yl, CONH2 and derivs., OH and derivs., NO2, CN, N3, NH2 and derivs., (un)substituted Ph, heterocyclyl, heteroaryl, etc.; m, n = independently 0-5; , and pharmaceutically acceptable salts, solvates or physiol. functional derivs. thereof] were prepared as Polo-like kinases (Plk) inhibitors. For example, II was prepared by cyclization of N-[(1S)-1-[3-[(3,4,5-trimethoxyphenyl)amino]-1,2,4-triazin-6-yl]ethyl]benzamide (preparation given) in 1,2-dichloroethane in the presence of POCl3. I were tested for inhibition of Plk1 and methylene blue growth. Thus, I and their pharmaceutical compns. are useful for the treatment of Plk-mediated conditions and a susceptible neoplasm, such as breast cancer, colon cancer, lung cancer, prostate cancer, lymphoma, leukemia, endometrial cancer, melanoma, ovarian cancer, pancreatic cancer, squamous carcinoma, carcinoma of the head and neck, and esophageal carcinoma (no data).

IT **774461-86-8P**, 5-Methyl-7-[3-(1H-pyrazol-4-ylethynyl)phenyl]-N-(3,4,5-trimethoxyphenyl)imidazo[5,1-f][1,2,4]triazin-2-amine
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(Plk1 inhibitor; preparation of imidazotriazines as Polo-like kinases inhibitors for treating cancers)

RN 774461-86-8 CAPLUS

CN Imidazo[5,1-f][1,2,4]triazin-2-amine, 5-methyl-7-[3-(1H-pyrazol-4-ylethynyl)phenyl]-N-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 6 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:769026 CAPLUS
DOCUMENT NUMBER: 141:423946
TITLE: First acetylenic derivatives of stable 3-imidazoline nitroxides
AUTHOR(S): Vasilevsky, Sergei F.; Klyatskaya, Svetlana V.; Korovnikova, Olga L.; Stass, Dmitri V.; Amitina, Svetlana A.; Grigir'ev, Igor A.; Elguero, Jose
CORPORATE SOURCE: Institute of Chemical Kinetics and Combustion, Siberian Branch of the Russian Academy of Science, Novosibirsk, 630090, Russia
SOURCE: Tetrahedron Letters (2004), 45(41), 7741-7743
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

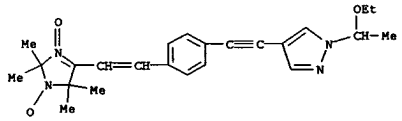
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The Stephens-Castro reaction of copper(I) salts of 1-aryl(hetaryl)alkynes with 2,2,5,5-tetramethyl-4-[2-(4-iodophenyl)-vinyl]imidazoline-3-oxide-1-ol proved to be a general method for the preparation of 2,2,5,5-tetramethyl-4-[2-(p-aryl(hetaryl)ethynylphenyl)]vinyl-3-imidazoline-3-oxide-1-oxyls (I; Ph,C6H4OCH2, 4-MeOC6H4,2-pyridyl; II, and III).

IT **792953-21-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and ESR of acetylenic derivs. of stable imidazoline nitroxides)

RN 792953-21-0 CAPLUS

CN 1H-Imidazol-1-yloxy, 2,5-dihydro-4-[2-[4-[[1-(1-ethoxyethyl)-1H-pyrazol-4-yl]ethynyl]phenyl]ethenyl]-2,2,5,5-tetramethyl-, 3-oxide (9CI) (CA INDEX NAME)



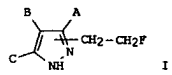
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:652635 CAPLUS
DOCUMENT NUMBER: 141:152555
TITLE: Preparation of insecticidal and acaricidal fluoroethylpyrazoles
INVENTOR(S): Park, Sheldon B.; Dekeyser, Mark A.; Mcdonald, Paul T.
PATENT ASSIGNEE(S): Crompton Co., USA; Uniroyal Chemical Co., Inc.
SOURCE: U.S. Pat. Appl. Publ., 10 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004157892	A1	20040812	US 2003-365762	20030212
PRIORITY APPLN. INFO.:			US 2003-365762	20030212

OTHER SOURCE(S): MARPAT 141:152555
GI



I

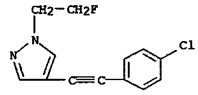
AB The fluoroethylpyrazole derivs. I wherein A and C are independently selected from the group consisting of hydrogen, nitro, carboxyalkyl, and carboxyhaloalkyl and B is selected from the group consisting of hydrogen, nitro, arylalkynyl, 5-membered heterocycle, and 6-membered heterocycle; provided that if A and C are hydrogen, B is arylalkynyl where aryl is Ph optionally substituted with halo, haloalkyl, alkyl, alkoxy, cyano, a six-membered heterocycle optionally substituted with halo, or a five-membered heterocycle optionally substituted with halo, a 5-membered heterocycle substituted with halo, alkyl, haloalkyl or carboxyalkyl; or 6-membered heterocyclyl substituted with halo. If B is hydrogen, A and C are independently selected from the group consisting of nitro, carboxyalkyl, and carboxyhaloalkyl; and if B is nitro, A and C are independently selected from the group consisting of hydrogen, carboxyalkyl, and carboxyhaloalkyl. These compds. are useful as insecticides and acaricides.

IT **730962-67-1P 730962-68-2P**
RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation as insecticide and acaricide)

RN 730962-67-1 CAPLUS

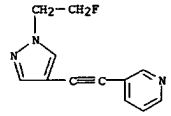
CN 1H-Pyrazole, 4-[(4-chlorophenyl)ethynyl]-1-(2-fluoroethyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 7 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 730962-68-2 CAPLUS

CN Pyridine, 3-[[1-(2-fluoroethyl)-1H-pyrazol-4-yl]ethynyl]- (9CI) (CA INDEX NAME)

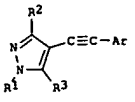


instant app

L4 ANSWER 8 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:589214 CAPLUS
DOCUMENT NUMBER: 141:101567
TITLE: Preparation of pyrazolylarylalkynes as insecticides and acaricides
INVENTOR(S): Ebenbeck, Wolfgang; Rampf, Florian; Marhold, Albrecht
PATENT ASSIGNEE(S): Germany
SOURCE: U.S. Pat. Appl. Publ., 12 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

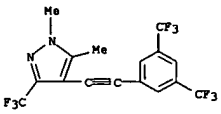
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004142820	A1	20040722	US 2004-751622	20040105
DE 10361426	A1	20040805	DE 2003-10361426	20031230
JP 2004210790	A2	20040729	JP 2004-1555	20040107
PRIORITY APPLN. INFO.:			DE 2003-10300123 A	20030107
OTHER SOURCE(S):		CASREACT 141:101567; MARPAT 141:101567		

GI

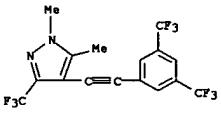


I

AB The pyrazolylarylalkynes I (R1 = H, alkyl, aralkyl, aryl, fluoroalkyl, etc.; R2, R3 = H, alkyl, alkoxy, aryl, aryloxy, etc.; Ar, carbocyclyl or heterocyclyl) are prepared as insecticides and acaricides. Intermediates for the preparation of I are prepared
IT 721401-78-1P
RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation as insecticide and acaricide)
RN 721401-78-1 CAPLUS
CN 1H-Pyrazole, 4-[[3,5-bis(trifluoromethyl)phenyl]ethynyl]-1,5-dimethyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 9 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
agrochems.)
RN 721401-78-1 CAPLUS
CN 1H-Pyrazole, 4-[[3,5-bis(trifluoromethyl)phenyl]ethynyl]-1,5-dimethyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 9 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:568166 CAPLUS
DOCUMENT NUMBER: 141:106468
TITLE: Preparation of pyrazolylalkynes from 4-acetylpyrazoles
INVENTOR(S): Ebenbeck, Wolfgang; Rampf, Florian; Marhold, Albrecht
PATENT ASSIGNEE(S): Bayer Chemicals A.-G., Germany
SOURCE: Ger. Offen., 13 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10361423	A1	20040715	DE 2003-10361423	20031230
US 2004229929	A1	20041118	US 2004-751761	20040105
JP 2004210789	A2	20040729	JP 2004-1263	20040106
PRIORITY APPLN. INFO.:			DE 2003-10300122 A1	20030107
OTHER SOURCE(S):		CASREACT 141:106468; MARPAT 141:106468		

GI

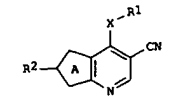
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention concerns pyrazolyl alkynes I [R1 = H, C1-12-alkyl, C5-14-aryl, C6-15-arylalkyl, C1-12-fluoroalkyl, (C1-8-alkylene)-BDE; R23 = H, C1-12-alkyl, C1-12-alkoxy, C5-14-aryl, C5-14-aryloxy, C6-15-arylalkyl, C6-15-arylalkoxy, Cl, F, CN, CHO, C1-12-fluoroalkyl, C1-12-fluoroalkylthio, C1-12-fluoroalkoxy, ABDE, AE, ASO2E, ABSO2R5, ASO3W, ACOW; A = C1-8-alkylene, C1-8-alkenylene, C1-8-fluoroalkylene; B O, S, NR4; R4 = H, C1-12-alkyl, C5-14-aryl, C6-15-arylalkyl; D = C:O, E = R5, OR5, NHR6, N(R6)2; R5 = C1-12-alkyl, C5-14-aryl, C6-15-arylalkyl; R6 = C1-12-alkyl, C5-14-aryl, C6-15-arylalkyl; N(R6)2 = C4-12-heterocycle; W = OH, NH2, OM; M = alkali metal ion, earth alkaline metal, NH4+, organic ammonium;
Ar = mono-, bi-, tricyclic aromatic with 5 -18 ring atoms, optionally containing
one or more N, O, S], a procedure for their production, as well as intermediates, and their use. Their preparation is characterized by halogenation of acetylpyrazole II, dehydrohalogenation of (1,1-dihaloethyl)pyrazole III or of (1-halovinyl)pyrazole IV and coupling of ethynylpyrazole V with Hal-Ar (Hal = I, Br, Cl) in the presence of a catalyst and a base, NHm(R11)(3-m) [m = 0, 1, 2; R11 = C1-12-alkyl, C5-14-aryl, C6-15-cycloalkyl; N(R11)2 = mono-, bi-, tricyclic heterocycle containing 4 to 8 carbons, heteroarom.]. Thus, I [R1 = R3 = Me, R2 = CF3, Ar = C6H3(CF3)2-3,5] was prepared in 91% yield from MeNHNH2 via cyclocondesation with (CF2CO)2O and MeOCMe:CH2, to give 1,5-Dimethyl-3-(trifluoromethyl)-1H-pyrazole (VI), which is acetylated with Ac2O, halogenated with PCl5, dehydrohalogenated with KOH in H2O and the resulting V (R1 = R3 = Me, R2 = CF3) was coupled with BrC6H3(CF3)2-3,5 in the presence of Pd(OAc)2, PPh3, CuI and Et2NH. I have agrochem. applications as insecticides or acaricides (no data).
IT 721401-78-1P, 3,5-Bis(trifluoromethyl)-1-[(1,5-dimethyl-3-(trifluoromethyl)-1H-pyrazol-4-yl)ethynyl]benzene
RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolylalkynes from 4-acetylpyrazoles for use as

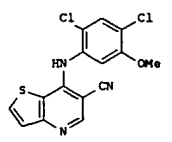
L4 ANSWER 10 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:467898 CAPLUS
DOCUMENT NUMBER: 141:23514
TITLE: Preparation of thieno[3,2-b]pyridine-6-carbonitriles and thieno[2,3-b]pyridine-5-carbonitriles as protein kinase, in particular protein tyrosine kinase, inhibitors
INVENTOR(S): Boschelli, Diane Harris; Zhang, Nan; Barrios Sosa, Ana Carolina; Durutlic, Haris; Wu, Biqi
PATENT ASSIGNEE(S): Wyeth, John, and Brother Ltd., USA
SOURCE: PCT Int. Appl., 188 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004048386	A2	20040610	WO 2003-US36206	20031114
WO 2004048386	A3	20041007		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRIORITY APPLN. INFO.:			US 2002-428862P P	20021125
OTHER SOURCE(S):		MARPAT 141:23514		

GI



I



II

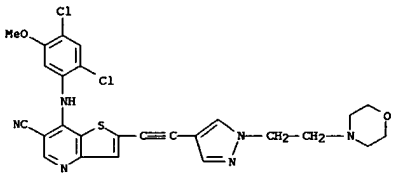
L4 ANSWER 10 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

AB Title compds. I [wherein X = NH and derivs., O, S(O)m, NHCH2; m = 0-2; R1 = (un)substituted Ph; R2 = H, CHO, F, Cl, Br, I, R3, C(:O)XR3; R3 = (un)asubstituted alkyl, cis-alkenyl, trans-alkenyl, alkynyl, hetero/aryl; A = thiophene ring giving a [3,2-b] or [2,3-b] fusion with the pyridine ring; their S-oxides, S-dioxides, and pharmaceutically acceptable salts] were prepared as protein kinase, in particular protein tyrosine kinase, inhibitors. Four biol. assays are given. For example, I was prepared by amination of 7-chlorothieno[3,2-b]pyridine-6-carbonitrile (preparation given) with 2,4-dichloro-5-methoxyaniline in THF in the presence of NaH at reflux. Selected I displayed IC50 values in the range of 7.3-58 nM for the inhibition of human Src kinase. Thus, I are useful in the treatment of neoplasm, stroke, osteoporosis, polycystic kidney disease, autoimmune disease, rheumatoid arthritis, and transplant rejection.

IT **700845-03-0P**, 7-[(2,4-Dichloro-5-methoxyphenyl)amino]-2-[[1-[2-(morpholin-4-yl)ethyl]-1H-pyrazol-4-yl]ethynyl]thieno[3,2-b]pyridine-6-carbonitrile **700845-69-8P**, 7-[(2,4-Dichloro-5-methoxyphenyl)amino]-2-[[1-(2-hydroxyethyl)-1H-pyrazol-4-yl]ethynyl]thieno[3,2-b]pyridine-6-carbonitrile
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of thieno[3,2-b]pyridine carbonitriles as protein kinase inhibitors)

RN 700845-03-0 CAPLUS

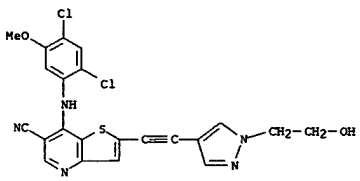
CN Thieno[3,2-b]pyridine-6-carbonitrile, 7-[(2,4-dichloro-5-methoxyphenyl)amino]-2-[[1-[2-(4-morpholinyl)ethyl]-1H-pyrazol-4-yl]ethynyl]- (9CI) (CA INDEX NAME)



RN 700845-69-8 CAPLUS

CN Thieno[3,2-b]pyridine-6-carbonitrile, 7-[(2,4-dichloro-5-methoxyphenyl)amino]-2-[[1-(2-hydroxyethyl)-1H-pyrazol-4-yl]ethynyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 10 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

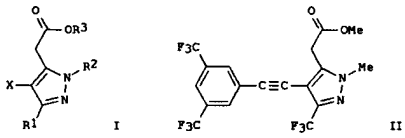


L4 ANSWER 11 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:267307 CAPLUS
DOCUMENT NUMBER: 140:303660
TITLE: Process for preparation of arylethynylpyrazole derivatives
INVENTOR(S): Urata, Takao; Sumitani, Naoko; He, Liangyou
PATENT ASSIGNEE(S): Agro-Kanesho Co., Ltd., Japan
SOURCE: PCT Int. Appl., 24 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004026839	A1	20040401	WO 2003-JP12012	20030919
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2004107264	A2	20040408	JP 2002-272480	20020919

PRIORITY APPLN. INFO.: JP 2002-272480 A 20020919
OTHER SOURCE(S): CASREACT 140:303660; MARPAT 140:303660
GI



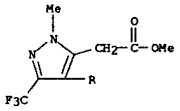
AB This invention pertains to a method for producing arylethynylpyrazole derivs. with general formula of I [R1 = H, halo, (un)substituted alkyl, alkenyl, alkynyl, alkoxy, or aryl; R2 = H, alkyl, haloalkyl, or (un)substituted aryl; R3 = alkyl, aralkyl, or aryl; X = halo], which comprises the coupling reaction of a halogenated pyrazole compound with an arylacetylene compound in the presence of a copper halide catalyst and a base. For example, 3,5-bis(trifluoromethyl)phenylacetylene (preparation given) was coupled with 1-methyl-4-iodo-3-trifluoromethylpyrazole-5-acetic acid Me ester (preparation given) in DMF in the presence of CuI and K2CO3 to give II (72%) with 98.6% purity. This invention provides a method to enable the coupling reaction at low cost with easy operation.

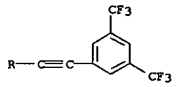
IT **331237-49-1P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

L4 ANSWER 11 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
(prepn. of arylethynylpyrazole derivs. via coupling reaction)

RN 331237-49-1 CAPLUS

CN 1H-Pyrazole-5-acetic acid, 4-[[3,5-bis(trifluoromethyl)phenyl]ethynyl]-1-methyl-3-(trifluoromethyl)-, methyl ester (9CI) (CA INDEX NAME)



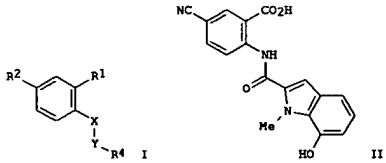


REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:182843 CAPLUS
DOCUMENT NUMBER: 140:235498
TITLE: Preparation of antibacterial benzoic acid derivatives
INVENTOR(S): Thorarensen, Atli; Ruble, Craig J.; Fisher, Jed F.; Romero, Donna L.; Beauchamp, Thomas J.; Northuis, Jill M.
PATENT ASSIGNEE(S): Pharmacia & Upjohn Company, USA
SOURCE: PCT Int. Appl., 500 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004018428	A1	20040304	WO 2003-US24796	20030822
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004110802	A1	20040610	US 2003-645802	20030820
PRIORITY APPLN. INFO.:			US 2002-405429P P	20020823
			US 2002-430592P P	20021203

OTHER SOURCE(S): MARPAT 140:235498
GI



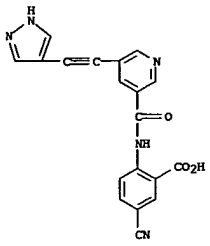
I II

AB Title compds. I [X = NH; Y = CO, CS, C(NCN), or X and Y together form an alkene or cycloalkyl; R1 = CO2H; R2 = electron withdrawing group; R4 = (un)substituted heterocycle, provided that the heterocycle is not simultaneously substituted with a sulfonamide and a urea or thiourea] and their pharmaceutically acceptable salts are prepared and disclosed as antibacterial agents. Thus, e.g., II was prepared via conversion of 7-(benzyloxy)-1-methyl-1H-indole-2-carboxylic acid (preparation given) to the acid chloride which is reacted with tert-butyl-2-amino-5-cyanobenzoate then subjected to hydrolysis. For compds. of the invention, the min.

L4 ANSWER 12 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
inhibitory concn. was detd. and found to correspond to a range of 0.0075 - >128 μg/mL. The invention provides antimicrobial agents and methods of using the agents for sterilization, sanitation, antisepsis, disinfection, and treatment of infections in mammals.

IT 668976-81-6P
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzoic acid derivs. as antibacterial agents)

RN 668976-81-6 CAPLUS
CN Benzoic acid, 5-cyano-2-[[[5-(1H-pyrazol-4-ylethynyl)-3-pyridinyl]carbonyl]amino]- (9CI) (CA INDEX NAME)

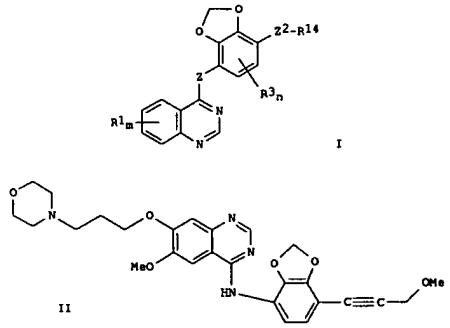


REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 13 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:41281 CAPLUS
DOCUMENT NUMBER: 140:94060
TITLE: Preparation of benzodioxole-containing quinazolines with MAP kinase inhibitory activity for treatment of cancer
INVENTOR(S): Hennequin, Laurent Francois Andre; Foote, Kevin Michael; Gibson, Keith Hopkinson
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; Astrazeneca UK Limited
SOURCE: PCT Int. Appl., 173 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004004732	A1	20040115	WO 2003-GB302874	20030704
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRIORITY APPLN. INFO.:			GB 2002-15825 A	20020709
			GB 2003-12897 A	20030605

OTHER SOURCE(S): MARPAT 140:94060
GI



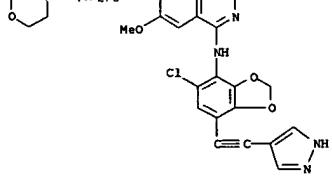
I II

L4 ANSWER 13 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

AB The invention concerns benzodioxole-containing quinazolines (shown as I; variables defined below; e.g. II), processes for their preparation, pharmaceutical compns. containing them and their use in the manufacture of a medicament for use as an anti-invasive or anti-proliferative agent in the containment and/or treatment of solid tumor disease (no data). Compds. I possess p44MAP kinase inhibitory activity (no data). Methods of preparation are claimed and .apprx.90 example prepns. are included. For example, II was prepared from N-(7-iodo-1,3-benzodioxol-4-yl)-6-methoxy-7-[3-(morpholin-4-yl)propoxy]quinazolin-4-amine and Me propargyl ether in the presence of bis(triphenylphosphine)palladium(II) chloride, copper iodide and iPr2NH in EtOAc; prepns. of the reactants are also described. For I: Z is O, S, SO, SO2, N(R2) or C(R2)2 (R2 is H or (1-6C)alkyl); m is 0-4; each R1 = halo, trifluoromethyl, cyano, isocyano, nitro, hydroxy, mercapto, amino, formyl, carboxy, carbamoyl, (1-6C)alkyl, (2-8C)alkenyl, (2-8C)alkynyl, etc. N = 0-2; R3 = halo, trifluoromethyl, cyano, nitro, hydroxy, amino, carboxy, carbamoyl, (1-6C)alkyl, (2-8C)alkenyl, (2-8C)alkynyl, (1-6C)alkoxy, etc.; Z2 is C.tplbond.C or C(R13):C(R13) (R13 is H or (1-6C)alkyl); and R14 = halo, cyano, isocyano, formyl, carboxy, (2-8C)alkenyl, (2-8C)alkynyl, (1-6C)alkoxycarbonyl, etc.; addnl. details are given in the claims.

IT 643085-62-5P, N-[5-Chloro-7-[(1H-pyrazol-4-yl)ethynyl]-1,3-benzodioxol-4-yl]-6-methoxy-7-[3-(morpholin-4-yl)propoxy]quinazolin-4-amine
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of benzodioxole-containing quinazolines with MAP kinase inhibitory activity for treatment of cancer)

RN 643085-62-5 CAPLUS
CN 4-Quinazolinamine, N-[5-chloro-7-(1H-pyrazol-4-ylethynyl)-1,3-benzodioxol-4-yl]-6-methoxy-7-[3-(4-morpholinyl)propoxy]- (9CI) (CA INDEX NAME)

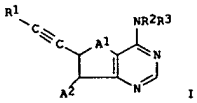


REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 14 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:511153 CAPLUS
DOCUMENT NUMBER: 139:69281
TITLE: Preparation of alkynyl thienopyrimidines as protein tyrosine kinase inhibitors useful against cancer and other disorders
INVENTOR(S): Caferro, Thomas R.; Chamberlain, Stanley Dawes; Donaldson, Kelly Horne; Harris, Philip Anthony; Gaul, Michael David; Uehling, David Edward; Vanderwall, Dana Edward
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 240 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003053446	A1	20030703	WO 2002-US39872	20021213
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1463507	A1	20041006	EP 2002-805582	20021213
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
US 2005009845	A1	20050113	US 2004-499247	20040617
PRIORITY APPLN. INFO.:			US 2001-342207P P	20011219
			WO 2002-US39872 W	20021213

OTHER SOURCE(S): MARPAT 139:69281
GI



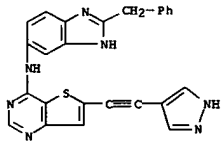
I

AB The present invention relates to alkynyl thienopyrimidines (shown as I; variables defined below; e.g. N-(2-benzyl-1H-benzimidazol-5-yl)-6-ethynylthieno[3,2-d]pyrimidin-4-amine), salts thereof, as well as use and preparation of the same. These compds. are inhibitors of various protein tyrosine kinases (PTKs) of the ErbB family and consequently are useful in the treatment of disorders mediated by aberrant activity of such kinases. Semiquant. pIC50 values for inhibition of ErbB-2 tyrosine kinase and IC50 values for cytotoxicity for HFF as a representative human normal cell line are reported for 11 examples of I. For I: one of A1 and A2 is S and the other is CH; R1 is H or -(CR11R11)n-R5; R2 is H or OC1-6alkyl; R3 = aryl

L4 ANSWER 14 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
(un)substituted with ≥1 halo, alkynyl, -CF3, -(CH2)nOR4, -(CH2)nSR4, -NO2, C1-6alkyl, -CN, -SO2R9, -(CH2)naryl and -(CH2)nNR9R10, and heteroaryl (un)substituted with ≥1 halo, alkynyl, -CF3, -(CH2)nOR4, -(CH2)nSR4, -NO2, C1-6alkyl, -CN, -SO2R9, -(CH2)naryl and -(CH2)nNR9R10; n = 0-6; addnl. details are given in the claims. Although the methods of prepn. are not claimed, .apprx.120 example prepns. of I are included.

IT 552295-40-6P, N-(2-Benzyl-1H-benzimidazol-5-yl)-6-[(1H-pyrazol-4-yl)ethynyl]thieno[3,2-d]pyrimidin-4-amine
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of alkynyl thienopyrimidines as protein tyrosine kinase inhibitors useful against cancer and other disorders)

RN 552295-40-6 CAPLUS
CN Thieno[3,2-d]pyrimidin-4-amine, N-[2-(phenylmethyl)-1H-benzimidazol-5-yl]-6-(1H-pyrazol-4-ylethynyl)- (9CI) (CA INDEX NAME)



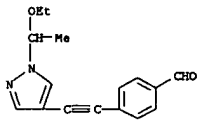
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:297061 CAPLUS
DOCUMENT NUMBER: 139:180009
TITLE: Ethyl vinyl ether - an agent for protection of the pyrazole NH-fragment. A convenient method for the preparation of N-unsubstituted 4-alkynylpyrazoles
AUTHOR(S): Vasilevsky, Sergei F.; Klyatskaya, Svetlana V.; Tretyakov, Eugene V.; Elguero, Jose
CORPORATE SOURCE: Institute of Chemical Kinetics and Combustion, Novosibirsk, 630090, Russia
SOURCE: Heterocycles (2003), 60(4), 879-886
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:180009

AB N-Unsubstituted 4-iodopyrazole is easily converted to 4-alkynyl derivs. in moderate to good overall yields by using intermediate protection of the nitrogen atom of the pyrazole ring by Et vinyl ether.

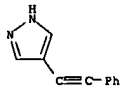
IT 575452-24-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(Et vinyl ether for protection of pyrazole NH-fragment and preparation of N-unsubstituted 4-alkynylpyrazoles)

RN 575452-24-3 CAPLUS
CN Benzaldehyde, 4-[[1-(1-ethoxyethyl)-1H-pyrazol-4-yl]ethynyl]- (9CI) (CA INDEX NAME)



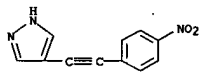
IT 82099-93-2P 444336-07-6P 575452-25-4P 575452-28-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(Et vinyl ether for protection of pyrazole NH-fragment and preparation of N-unsubstituted 4-alkynylpyrazoles)

RN 82099-93-2 CAPLUS
CN 1H-Pyrazole, 4-(phenylethynyl)- (9CI) (CA INDEX NAME)

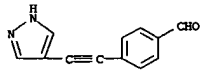


RN 444336-07-6 CAPLUS
CN 1H-Pyrazole, 4-[(4-nitrophenyl)ethynyl]- (9CI) (CA INDEX NAME)

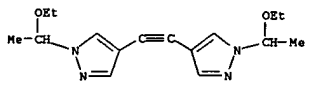
L4 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 575452-25-4 CAPLUS
CN Benzaldehyde, 4-(1H-pyrazol-4-ylethynyl)- (9CI) (CA INDEX NAME)

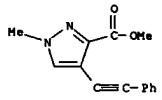


RN 575452-28-7 CAPLUS
CN 1H-Pyrazole, 4,4'-(1,2-ethynediyl)bis[1-(1-ethoxyethyl)- (9CI) (CA INDEX NAME)

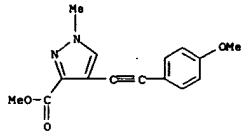


REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 16 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:61754 CAPLUS
DOCUMENT NUMBER: 138:368802
TITLE: Study of the heterocyclization of vic-substituted hydrazides of acetylenylpyrazolecarboxylic acids into N-aminopyrazolopyridinones
AUTHOR(S): Vasilevsky, Sergei F.; Mshvidobadze, Elena V.; Elguero, Jose
CORPORATE SOURCE: Institute of Chemical Kinetics and Combustion, Siberian Branch of the Russian Academy of Sciences, Novosibirsk, 630090, Russia
SOURCE: Journal of Heterocyclic Chemistry (2002), 39(6), 1229-1233
CODEN: JHTCAD; ISSN: 0022-152X
PUBLISHER: HeteroCorporation
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:368802
AB The authors report a new and efficient methodol. to prepare N-aminopyrazolo[4,3-c]pyridin-4-ones and N-aminopyrazolo[3,4-c]pyridin-4-ones from vic-acetylenyl/hydrazido pyrazoles. The procedure involves the intermediate synthesis of Me esters of acetylenylpyrazole carboxylic acids and the subsequent cyclization under a variety of conditions.
IT **79229-73-5P 521944-76-3P 521944-81-0P**
521944-82-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-aminopyrazolopyridinones by heterocyclization of vic-substituted hydrazides of acetylenylpyrazolecarboxylic acids)
RN 79229-73-5 CAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 1-methyl-4-(phenylethynyl)-, methyl ester (9CI) (CA INDEX NAME)

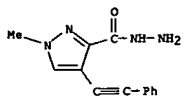


RN 521944-76-3 CAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 4-[(4-methoxyphenyl)ethynyl]-1-methyl-, methyl ester (9CI) (CA INDEX NAME)

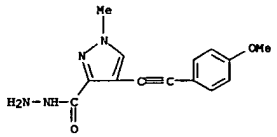


RN 521944-81-0 CAPLUS

L4 ANSWER 16 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN 1H-Pyrazole-3-carboxylic acid, 1-methyl-4-(phenylethynyl)-, hydrazide (9CI) (CA INDEX NAME)

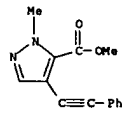


RN 521944-82-1 CAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 4-[(4-methoxyphenyl)ethynyl]-1-methyl-, hydrazide (9CI) (CA INDEX NAME)

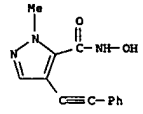


REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 17 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:955146 CAPLUS
DOCUMENT NUMBER: 138:338044
TITLE: Heterocyclization of vic-substituted hydroxamic acid salts of acetylenylpyrazoles. A new procedure for the preparation of pyrazolo[3,4-c]pyridin-7-ones
AUTHOR(S): Vasilevsky, Sergei F.; Mshvidobadze, Elena V.; Elguero, Jose
CORPORATE SOURCE: Institute of Chemical Kinetics and Combustion, Siberian Branch of the Russian Academy of Sciences, Novosibirsk, 630090, Russia
SOURCE: Heterocycles (2002), 57(12), 2255-2260
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:338044
AB Procedures for the preparation of 5-substituted pyrazolo[3,4-c]pyridin-7-ones and 5-substituted 6-hydroxypyrazolo[3,4-c]pyridin-7-ones were developed based on heterocyclization of vic-acetylenylpyrazolylhydroxamic acids under the influence of copper(I) salts in DMF or with organic bases in butanol or methanol.
IT **79229-75-7P 518036-11-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrazolo[3,4-c]pyridin-7-ones by heterocyclization of vic-substituted hydroxamic acid of acetylenylpyrazoles using copper(I) chloride catalyst)
RN 79229-75-7 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 1-methyl-4-(phenylethynyl)-, methyl ester (9CI) (CA INDEX NAME)



RN 518036-11-8 CAPLUS
CN 1H-Pyrazole-5-carboxamide, N-hydroxy-1-methyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

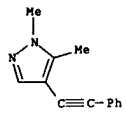
L4 ANSWER 17 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

L4 ANSWER 18 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:117129 CAPLUS
DOCUMENT NUMBER: 137:125114
TITLE: Synthesis of unsymmetrical hetaryl-1,2-diketones
AUTHOR(S): Yusubov, Mekhman S.; Zholobova, Galina A.; Vasilevsky, Sergey F.; Tretyakov, Eugene V.; Knight, David W.
CORPORATE SOURCE: The Siberian Medical University, Tomsk, 634050, Russia
SOURCE: Tetrahedron (2002), 58(8), 1607-1610
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:125114

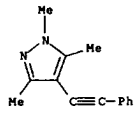
AB Oxidation of the triple bond in 4-alkynylpyrazoles and acetylenic derivs. of crown-ethers with PdCl2-DMSO was carried out to give unsym. hetaryl-1,2-diketones. Attempts to oxidize the triple bond in 5-alkynylpyrazole and alkynylpyridines failed.

IT **71443-54-4P**, 1,5-Dimethyl-4-phenylethynylpyrazole
444336-05-4P, 1,3,5-Trimethyl-4-(2-phenylethynyl)pyrazole
444336-06-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of unsym. hetaryl-1,2-diketones by oxidation of alkyne triple bonds)

RN 71443-54-4 CAPLUS
CN 1H-Pyrazole, 1,5-dimethyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)

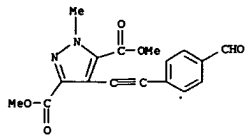


RN 444336-05-4 CAPLUS
CN 1H-Pyrazole, 1,3,5-trimethyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)



RN 444336-06-5 CAPLUS
CN 1H-Pyrazole-3,5-dicarboxylic acid, 4-[(4-formylphenyl)ethynyl]-1-methyl-, dimethyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 18 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



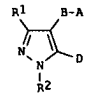
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 19 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:228652 CAPLUS
DOCUMENT NUMBER: 134:252335
TITLE: Preparation of pyrazole derivatives as insecticidal and acaricidal agents
INVENTOR(S): Oda, Masatsugu; Katsurada, Manabu; Shiga, Yasushi; Fukuchi, Toshiki; Kato, Taku
PATENT ASSIGNEE(S): Mitsubishi Chemical Corporation, Japan
SOURCE: PCT Int. Appl., 50 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001020993	A1	20010329	WO 2000-JP6479	20000921
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2383157	AA	20010329	CA 2000-2383157	20000921
AU 2000073191	A5	20010424	AU 2000-73191	20000921
EP 1219173	A1	20020703	EP 2000-961164	20000921
EP 1219173	B1	20040616		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
AT 268990	E	20040715	AT 2000-961164	20000921
ES 2218215	T3	20041116	ES 2000-961164	20000921
JP 2001158704	A2	20010612	JP 2000-287933	20000922
US 2002156115	A1	20021024	US 2002-103785	20020325
US 2003191171	A1	20031009	US 2002-331326	20021231

PRIORITY APPLN. INFO.: JP 1999-270861 A 19990924
WO 2000-JP6479 W 20000921
US 2002-103785 A3 20020325

OTHER SOURCE(S): MARPAT 134:252335
GI



I

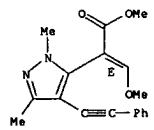
AB Insecticidal and acaricidal agents containing as the active ingredient pyrazolyl derivs. of general formula [I; A is hydrogen, (un)substituted alkyl, (un)substituted alkenyl, or (un)substituted alkynyl, trisubstituted silyl, (un)substituted aryl, or (un)substituted heterocyclic group; B is a single bond, -(G1)n-G2-(G1)m-, carbonyl, -CH2-O-N:C(R3)-, or -CH:N-O-(CR3R4)n-; wherein G1 is O, S, SO, or SO2; G2 is alkylene or

L4 ANSWER 19 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
alkenylene; R3 and R4 are hydrogen, alkyl or haloalkyl; n and m is an integer of 0 or 1; R1 is hydrogen, halogeno, (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkynyl, (un)substituted alkoxy, or (un)substituted aryl; R2 is hydrogen, alkyl, haloalkyl, or (un)substituted aryl; and D is -C(:Y)COX or -N(R5)CO2G5; wherein X is hydroxy, alkoxy, or alkylamino; Y is CH-(G3)n-G4 or N-O-G4; wherein G3 is O or S; G4 is alkyl or haloalkyl; n is integer of 0 or 1; R5 is alkyl, alkenyl, alkynyl, alkylthioalkyl, or alkoxyalkyl; G5 is alkyl] are described. Thus, 4-iodo-1,3-dimethylpyrazol-5-ylacetic acid iso-Pr ester was coupled with 3,5-bis(trifluoromethyl)phenylacetylene in the presence of Pd(PPh3)4 and CuI in Et3N under refluxing at 90° for 4 h to give 81% 2-[1,3-dimethyl-4-[3,5-bis(trifluoromethyl)phenylethynyl]-5-pyrazolyl]acetic acid iso-Pr ester. To a soln. of the latter acetate ester in Me formate was added a soln. of NaH in 1,2-dimethoxyethane and MeOH, stirred at room temp. for 2 h, treated with K2CO3, KI, and DMF, and stirred overnight to give 52% 2-[1,3-dimethyl-4-[3,5-bis(trifluoromethyl)phenylethynyl]-5-pyrazolyl]-3-(methoxy)acrylic acid iso-Pr ester, which at 500 ppm controlled 100% Plutella xylostella konaga larvae on cabbage leaves.

IT **153208-02-7P 153208-09-4P 331236-81-8P**
331236-82-9P 331236-83-0P 331236-84-1P
331236-85-2P 331236-86-3P 331236-87-4P
331236-88-5P 331236-89-6P 331236-90-9P,
(E)-2-(1,3-Dimethyl-4-(2-(4-(2-chloro-4-fluorophenoxy)phenyl)ethynyl)-1H-pyrazol-5-yl)-3-methoxy-2-propenoic acid methyl ester **331236-91-0P**
331236-92-1P 331236-93-2P 331236-94-3P
331236-95-4P 331236-96-5P 331236-97-6P
331236-98-7P 331236-99-8P 331237-00-4P
331237-01-5P 331237-02-6P 331237-03-7P
331237-04-8P 331237-05-9P 331237-06-0P
331237-07-1P 331237-08-2P 331237-09-3P
331237-10-6P 331237-11-7P 331237-12-8P
331237-13-9P 331237-14-0P 331237-15-1P
331237-16-2P 331237-17-3P 331237-18-4P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazole derivs. as insecticidal and acaricidal agents)

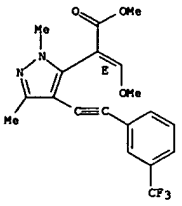
RN 153208-02-7 CAPLUS
CN 1H-Pyrazole-5-acetic acid, α-(methoxymethylene)-1,3-dimethyl-4-(phenylethynyl)-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



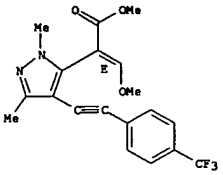
RN 153208-09-4 CAPLUS
CN 1H-Pyrazole-5-acetic acid, α-(methoxymethylene)-1,3-dimethyl-4-[[3-(trifluoromethyl)phenyl]ethynyl]-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



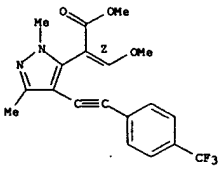
RN 331236-81-8 CAPLUS
CN 1H-Pyrazole-5-acetic acid, α-(methoxymethylene)-1,3-dimethyl-4-[[4-(trifluoromethyl)phenyl]ethynyl]-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

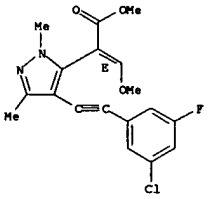
Double bond geometry as shown.



RN 331236-82-9 CAPLUS
CN 1H-Pyrazole-5-acetic acid, α-(methoxymethylene)-1,3-dimethyl-4-[[4-(trifluoromethyl)phenyl]ethynyl]-, methyl ester, (αZ)- (9CI) (CA INDEX NAME)

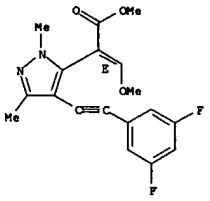
Double bond geometry as shown.





RN 331236-86-3 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[(3,5-difluorophenyl)ethynyl]-α-(methoxymethylene)-1,3-dimethyl-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

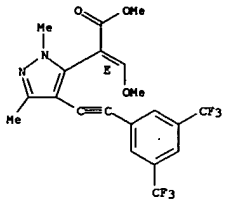


RN 331236-87-4 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[(3,5-dimethylphenyl)ethynyl]-α-(methoxymethylene)-1,3-dimethyl-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

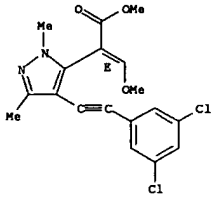
RN 331236-83-0 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[[3,5-bis(trifluoromethyl)phenyl]ethynyl]-α-(methoxymethylene)-1,3-dimethyl-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



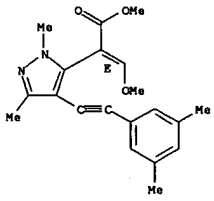
RN 331236-84-1 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[(3,5-dichlorophenyl)ethynyl]-α-(methoxymethylene)-1,3-dimethyl-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



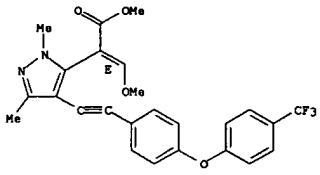
RN 331236-85-2 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[(3-chloro-5-fluorophenyl)ethynyl]-α-(methoxymethylene)-1,3-dimethyl-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



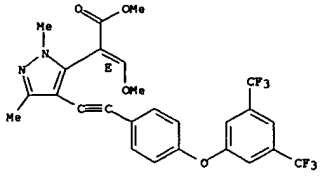
RN 331236-88-5 CAPLUS
CN 1H-Pyrazole-5-acetic acid, α-(methoxymethylene)-1,3-dimethyl-4-[[4-[4-(trifluoromethyl)phenoxy]phenyl]ethynyl]-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 331236-89-6 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[[4-[3,5-bis(trifluoromethyl)phenoxy]phenyl]ethynyl]-α-(methoxymethylene)-1,3-dimethyl-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

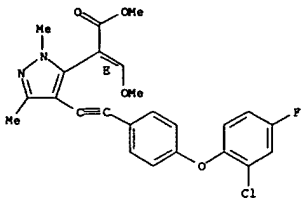
Double bond geometry as shown.



RN 331236-90-9 CAPLUS

CN 1H-Pyrazole-5-acetic acid, 4-[[4-(2-chloro-4-fluorophenoxy)phenyl]ethynyl]-α-(methoxymethylene)-1,3-dimethyl-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

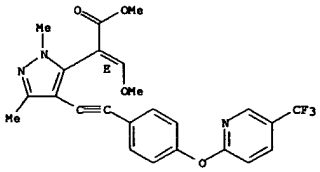
Double bond geometry as shown.



RN 331236-91-0 CAPLUS

CN 1H-Pyrazole-5-acetic acid, α-(methoxymethylene)-1,3-dimethyl-4-[[4-[[5-(trifluoromethyl)-2-pyridinyl]oxy]phenyl]ethynyl]-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

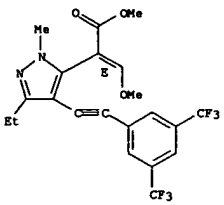
Double bond geometry as shown.



RN 331236-92-1 CAPLUS

CN 1H-Pyrazole-5-acetic acid, 4-[[3,5-bis(trifluoromethyl)phenyl]ethynyl]-3-ethyl-α-(methoxymethylene)-1-methyl-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

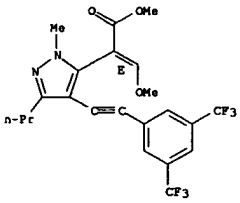
Double bond geometry as shown.



RN 331236-93-2 CAPLUS

CN 1H-Pyrazole-5-acetic acid, 4-[[3,5-bis(trifluoromethyl)phenyl]ethynyl]-α-(methoxymethylene)-1-methyl-3-propyl-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

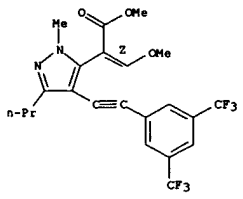
Double bond geometry as shown.



RN 331236-94-3 CAPLUS

CN 1H-Pyrazole-5-acetic acid, 4-[[3,5-bis(trifluoromethyl)phenyl]ethynyl]-α-(methoxymethylene)-1-methyl-3-propyl-, methyl ester, (αZ)- (9CI) (CA INDEX NAME)

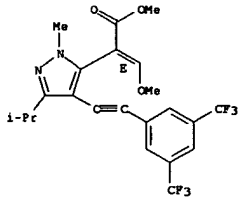
Double bond geometry as shown.



RN 331236-95-4 CAPLUS

CN 1H-Pyrazole-5-acetic acid, 4-[[3,5-bis(trifluoromethyl)phenyl]ethynyl]-α-(methoxymethylene)-1-methyl-3-(1-methylethyl)-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

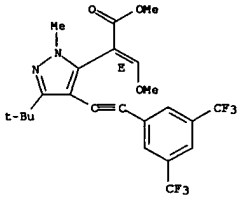
Double bond geometry as shown.



RN 331236-96-5 CAPLUS

CN 1H-Pyrazole-5-acetic acid, 4-[[3,5-bis(trifluoromethyl)phenyl]ethynyl]-3-(1,1-dimethylethyl)-α-(methoxymethylene)-1-methyl-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

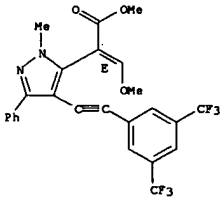
Double bond geometry as shown.



RN 331236-97-6 CAPLUS

CN 1H-Pyrazole-5-acetic acid, 4-[[3,5-bis(trifluoromethyl)phenyl]ethynyl]-α-(methoxymethylene)-1-methyl-3-phenyl-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

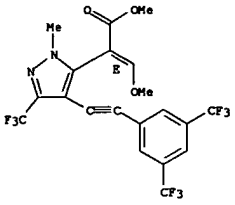
Double bond geometry as shown.



RN 331236-98-7 CAPLUS

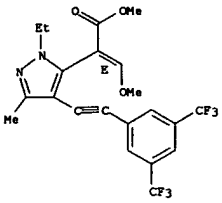
CN 1H-Pyrazole-5-acetic acid, 4-[[3,5-bis(trifluoromethyl)phenyl]ethynyl]-α-(methoxymethylene)-1-methyl-3-(trifluoromethyl)-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



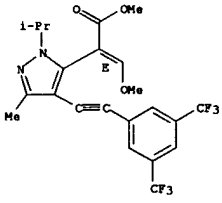
RN 331236-99-8 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[[3,5-bis(trifluoromethyl)phenyl]ethynyl]-1-ethyl-α-(methoxymethylene)-3-methyl-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



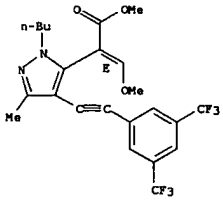
RN 331237-00-4 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[[3,5-bis(trifluoromethyl)phenyl]ethynyl]-1-ethyl-α-(methoxymethylene)-3-methyl-, methyl ester, (α2)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



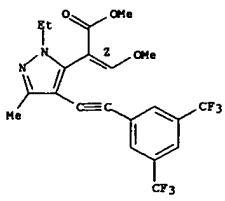
RN 331237-03-7 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[[3,5-bis(trifluoromethyl)phenyl]ethynyl]-1-butyl-α-(methoxymethylene)-3-methyl-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



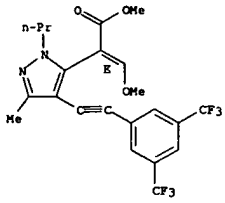
RN 331237-04-8 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[[3,5-bis(trifluoromethyl)phenyl]ethynyl]-1-(1,1-dimethylethyl)-α-(methoxymethylene)-3-methyl-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



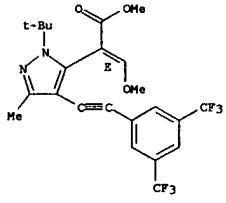
RN 331237-01-5 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[[3,5-bis(trifluoromethyl)phenyl]ethynyl]-α-(methoxymethylene)-3-methyl-1-propyl-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



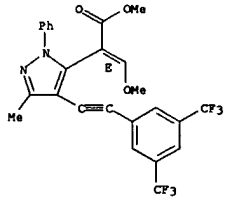
RN 331237-02-6 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[[3,5-bis(trifluoromethyl)phenyl]ethynyl]-α-(methoxymethylene)-3-methyl-1-(1-methylethyl)-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



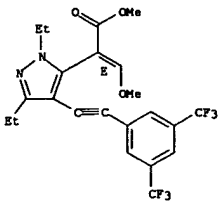
RN 331237-05-9 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[[3,5-bis(trifluoromethyl)phenyl]ethynyl]-α-(methoxymethylene)-3-methyl-1-phenyl-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



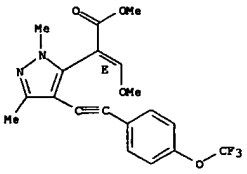
RN 331237-06-0 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[[3,5-bis(trifluoromethyl)phenyl]ethynyl]-1,3-diethyl-α-(methoxymethylene)-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



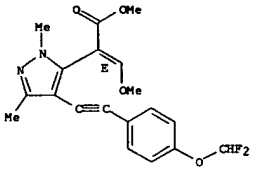
RN 331237-07-1 CAPLUS
CN 1H-Pyrazole-5-acetic acid, α-(methoxymethylene)-1,3-dimethyl-4-[[4-(trifluoromethoxy)phenyl]ethynyl]-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 331237-08-2 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[[4-(difluoromethoxy)phenyl]ethynyl]-α-(methoxymethylene)-1,3-dimethyl-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

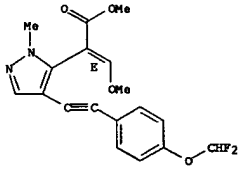
Double bond geometry as shown.



RN 331237-09-3 CAPLUS

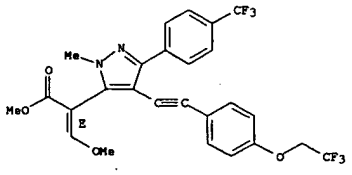
RN 331237-12-8 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[[4-(difluoromethoxy)phenyl]ethynyl]-α-(methoxymethylene)-1-methyl-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 331237-13-9 CAPLUS
CN 1H-Pyrazole-5-acetic acid, α-(methoxymethylene)-1-methyl-4-[[4-(2,2,2-trifluoroethoxy)phenyl]ethynyl]-3-[4-(trifluoromethyl)phenyl]-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

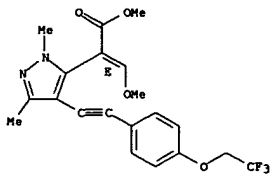


RN 331237-14-0 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[[3,5-bis(trifluoromethyl)phenyl]ethynyl]-α-(methoxymethylene)-1-methyl-3-[4-(trifluoromethyl)phenyl]-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

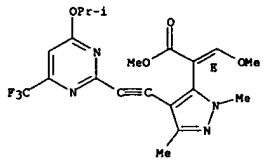
CN 1H-Pyrazole-5-acetic acid, α-(methoxymethylene)-1,3-dimethyl-4-[[4-(2,2,2-trifluoroethoxy)phenyl]ethynyl]-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



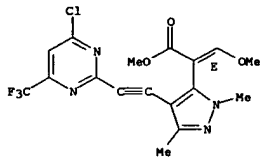
RN 331237-10-6 CAPLUS
CN 1H-Pyrazole-5-acetic acid, α-(methoxymethylene)-1,3-dimethyl-4-[[4-(1-methylethoxy)-6-(trifluoromethyl)-2-pyrimidinyl]ethynyl]-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

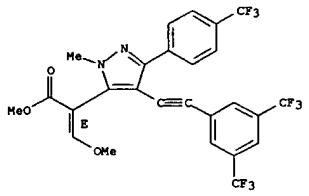
Double bond geometry as shown.



RN 331237-11-7 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[[4-chloro-6-(trifluoromethyl)-2-pyrimidinyl]ethynyl]-α-(methoxymethylene)-1,3-dimethyl-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

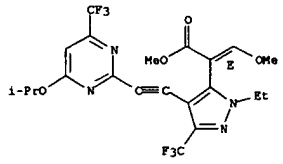
Double bond geometry as shown.





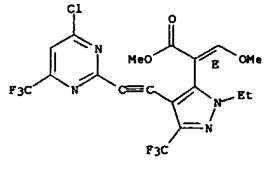
RN 331237-15-1 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 1-ethyl-α-(methoxymethylene)-4-[[4-(1-methylethoxy)-6-(trifluoromethyl)-2-pyrimidinyl]ethynyl]-3-(trifluoromethyl)-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 331237-16-2 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[[4-chloro-6-(trifluoromethyl)-2-pyrimidinyl]ethynyl]-1-ethyl-α-(methoxymethylene)-3-(trifluoromethyl)-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

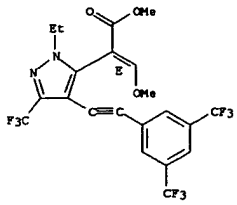
Double bond geometry as shown.



RN 331237-17-3 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[[3,5-bis(trifluoromethyl)phenyl]ethynyl]-1-ethyl-α-(methoxymethylene)-3-(trifluoromethyl)-, methyl ester,

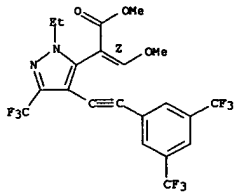
(αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

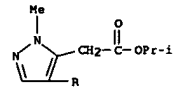


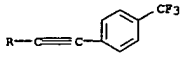
RN 331237-18-4 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[[3,5-bis(trifluoromethyl)phenyl]ethynyl]-1-ethyl-α-(methoxymethylene)-3-(trifluoromethyl)-, methyl ester, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

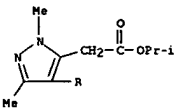


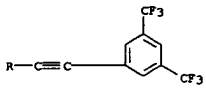
IT **331237-42-4P 331237-43-5P 331237-47-9P 331237-49-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrazole derivs. as insecticidal and acaricidal agents)
RN 331237-42-4 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 1-methyl-4-[[4-(trifluoromethyl)phenyl]ethynyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)



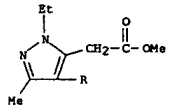


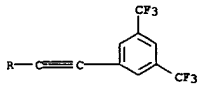
RN 331237-43-5 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[[3,5-bis(trifluoromethyl)phenyl]ethynyl]-1,3-dimethyl-, 1-methylethyl ester (9CI) (CA INDEX NAME)



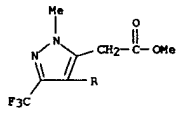


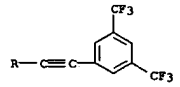
RN 331237-47-9 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[[3,5-bis(trifluoromethyl)phenyl]ethynyl]-1-ethyl-3-methyl-, methyl ester (9CI) (CA INDEX NAME)





RN 331237-49-1 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[[3,5-bis(trifluoromethyl)phenyl]ethynyl]-1-methyl-3-(trifluoromethyl)-, methyl ester (9CI) (CA INDEX NAME)



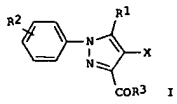


REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2000:412214 CAPLUS
DOCUMENT NUMBER: 133:30728
TITLE: Preparation of 1-phenylpyrazole-3-carboxamides as fungicides
INVENTOR(S): Okada, Itaru; Tomita, Hirofumi; Shiga, Yasushi
PATENT ASSIGNEE(S): Mitsubishi Chemical Industries Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 23 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
JP 2000169453	A2	20000620	JP 1999-254112		19990908
KR 2000023547	A	20000425	KR 1999-41921		19990930
PRIORITY APPLN. INFO.:			JP 1998-277585	A	19980930

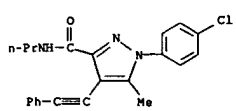
OTHER SOURCE(S): MARPAT 133:30728
GI



I

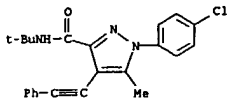
AB Title compds. I (R1 = H, alkyl, alkoxy; R2 = H, halo, alkyl; R3 = amino, alkylamino; X = halo, alkyl, allyl), useful as fungicides, are prepared Thus, reaction of 4-chlorophenylhydrazine hydrochloride with di-Et oxalylpropionate in EtOAc in the presence of NaOH gave Et 1-(4-chlorophenyl)-5-hydroxy-4-methylpyrazole-3-carboxylate, which was converted in several steps to 1-(4-chlorophenyl)-5-methoxy-4-methyl-N-propylpyrazole-3-carboxamide (II). II at 500 ppm showed fungicidal activity against Magnaporthe grisea.

IT **274254-22-7P 274254-23-8P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1-phenylpyrazole-3-carboxamides as fungicides)
RN 274254-22-7 CAPLUS
CN 1H-Pyrazole-3-carboxamide, 1-(4-chlorophenyl)-5-methyl-4-(phenylethynyl)-N-propyl- (9CI) (CA INDEX NAME)



RN 274254-23-8 CAPLUS

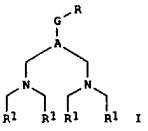
L4 ANSWER 20 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN 1H-Pyrazole-3-carboxamide, 1-(4-chlorophenyl)-N-(1,1-dimethylethyl)-5-methyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)



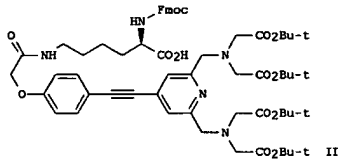
L4 ANSWER 21 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:819049 CAPLUS
DOCUMENT NUMBER: 132:64173
TITLE: Preparation of labeling reactants for fluorescent labeling of biospecific binding reactants
INVENTOR(S): Takalo, Harri; Hovinen, Jari; Mukkala, Veli-matti; Liitti, Pivi; Mikola, Heikki
PATENT ASSIGNEE(S): Wallac Oy, Finland
SOURCE: Eur. Pat. Appl., 26 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 967205	A1	19991229	EP 1999-660100	19990603
EP 967205	B1	20030917		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 6080839	A	20000627	US 1998-104219	19980625

PRIORITY APPLN. INFO.: US 1998-104219 A 19980625
OTHER SOURCE(S): CASREACT 132:64173; MARPAT 132:64173
GI



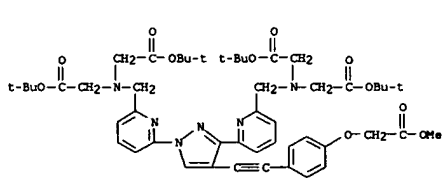
I



II

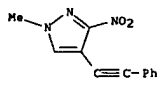
AB Novel pyridinediylbis(methylenenitrilo)tetrakisacetic acid labeling reactants, suitable for fluorescent labeling of biospecific binding reactants in solid-phase synthesis, were prepared The novel labeling reactants (I) [wherein A = a bivalent aromatic structure capable of absorbing
light or energy and transferring the excitation energy to a lanthanide ion after the product made by solid-phase synthesis has been released from the

L4 ANSWER 21 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
used solid support, deprotected, and converted to a lanthanide chelate; R = -Z(G1-NH-X)G2-E; X = a transient protecting group, e.g. 2-(4-nitrophenylsulfonyl)ethoxycarbonyl, trityl, 4-methoxytrityl, 4,4'-dimethoxytrityl, BOC, Fmoc; E = a carboxylic acid, its salt, active ester (e.g. N-hydroxysuccinimido, nitrophenol, 2,4-dinitrophenol, or pentafluorophenol), or halide; Z = the bridge point; G = a bridge between A and Z; G1 = a bridge between NH and Z; G2 = a bridge between E and Z; R1 = CO2R2; R2 = alkyl or (un)substituted Ph or benzyl] are particularly useful in the labeling of small mols. Thus, II was prepd. in a 4-step sequence involving (1) desilylation of Me (4-trimethylsilylethynylphenoxy) acetate (83%), (2) addn. to tetra(tert-Bu) 2,2',2'',2'''-[(4-bromopyridine-2,6-diyl)bis(methylenenitrilo)]tetrakis(acetate) (75%), (3) deesterification of the phenoxyacetate with KOH (67%), and (4) amidation with α-Fmoc-lysine.HCl (56%). II was used for labeling of an estradiol deriv., incorporating four Eu(III) chelates, on a solid support (no data).
IT **253137-97-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of pyridinediylbis(methylenenitrilo)tetrakisaceti
c acid labeling reactants for fluorescent labeling of biospecific binding reactants in solid phase synthesis)
RN 253137-97-2 CAPLUS
CN Glycine, N,N'-[[4-[[4-(2-methoxy-2-oxoethoxy)phenyl]ethynyl]-1H-pyrazole-1,3-diyl]bis(6,2-pyridinediylmethylene)]bis[N-[2-(1,1-dimethylethoxy)-2-oxoethyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

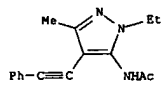


REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 22 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:781600 CAPLUS
DOCUMENT NUMBER: 132:237020
TITLE: Peculiarities of copper(I)- and palladium-catalyzed cross-coupling of terminal alkynes with vicinal amino- and (N-acetylamino)iodopyrazoles. Synthesis of alkynylaminopyrazoles
AUTHOR(S): Tretyakov, Eugene V.; Knight, David W.; Vasilevsky, Sergei F.
CORPORATE SOURCE: Institute of Chemical Kinetics and Combustion, Siberian Branch of the Russian Academy of Sciences, Novosibirsk, 630090, Russia
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1999), (24), 3713-3720
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:237020
AB A number of vicinal amino- and (N-acetylamino)alkylpyrazoles have been synthesized by cross-coupling reactions of iodopyrazoles with alk-1-ynes using a combination of Pd(PPh3)2Cl2 and CuI as catalyst in Et3N or with copper acetylides. The latter Stephens-Castro reaction of copper acetylides with these amino- and (N-acetylamino)iodopyrazoles was established as a common method for the preparation of (N-acetylamino)alkynylpyrazoles. The Pd/Cu-catalyzed cross-coupling of iodopyrazoles (Sonogashira reaction) with alk-1-ynes bearing electron-releasing substituents was unsuitable for the synthesis of alkynylpyrazoles: 3- and 5-iodopyrazoles were unreactive but, in the case of 4-iodo derivs., reductive deiodination, accompanied by homocoupling of the alk-1-yne component, was the only reaction.
IT **107879-57-2P 260442-52-2P 260442-53-3P 260442-56-6P 260442-58-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(copper(I)- and palladium-catalyzed cross-coupling of terminal alkynes with vicinal amino- and (N-acetylamino)iodopyrazoles)
RN 107879-57-2 CAPLUS
CN 1H-Pyrazole, 1-methyl-3-nitro-4-(phenylethynyl)- (9CI) (CA INDEX NAME)

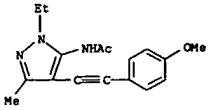


RN 260442-52-2 CAPLUS
CN Acetamide, N-[1-ethyl-3-methyl-4-(phenylethynyl)-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

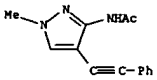


L4 ANSWER 22 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

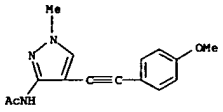
RN 260442-53-3 CAPLUS
CN Acetamide, N-[1-ethyl-4-[(4-methoxyphenyl)ethynyl]-3-methyl-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)



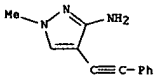
RN 260442-56-6 CAPLUS
CN Acetamide, N-[1-methyl-4-(phenylethynyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



RN 260442-58-8 CAPLUS
CN Acetamide, N-[4-[(4-methoxyphenyl)ethynyl]-1-methyl-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

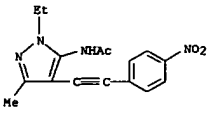


IT **220637-81-0P 260442-48-6P 260442-50-0P**
260442-66-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(copper(I)- and palladium-catalyzed cross-coupling of terminal alkynes with vicinal amino- and (N-acetylamino)iodopyrazoles)
RN 220637-81-0 CAPLUS
CN 1H-Pyrazol-3-amine, 1-methyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)

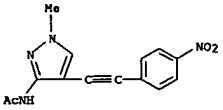


RN 260442-48-6 CAPLUS

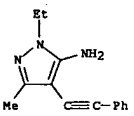
L4 ANSWER 22 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN Acetamide, N-[1-ethyl-3-methyl-4-[(4-nitrophenyl)ethynyl]-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)



RN 260442-50-0 CAPLUS
CN Acetamide, N-[1-methyl-4-[(4-nitrophenyl)ethynyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



RN 260442-66-8 CAPLUS
CN 1H-Pyrazol-5-amine, 1-ethyl-3-methyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)

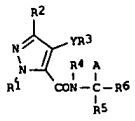


REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 23 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:595144 CAPLUS
DOCUMENT NUMBER: 131:214287
TITLE: Preparation of pyrazolecarboxamides as insecticides, acaricides, and fungicides
INVENTOR(S): Kano, Hiroki; Ikeda, Yoshiya; Kyomura, Nobuo; Tomita, Hirofumi; Fukuchi, Toshiki
PATENT ASSIGNEE(S): Mitsubishi Chemical Corporation, Japan
SOURCE: PCT Int. Appl., 61 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

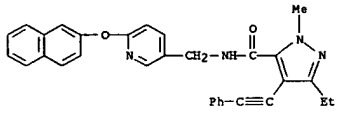
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9946247	A1	19990916	WO 1999-JP1160	19990310
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
JP 2002187882	A2	20020705	JP 1998-59510	19980311
AU 9927470	A1	19990927	AU 1999-27470	19990310
PRIORITY APPLN. INFO.:			JP 1998-59510 A	19980311
			WO 1999-JP1160 W	19990310

OTHER SOURCE(S): MARPAT 131:214287
GI



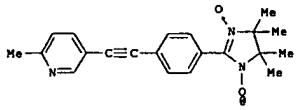
AB Title compds. I [R1, R2 = H, alkyl; R3 = H, halo, alkyl, etc.; R4 = H, alkyl, acyl, alkoxycarbonyl, alkoxyalkyl; R5, R6 = H, alkyl; A = (un)substituted Ph, 5- or 6-membered heterocyclyl; Y = a group containing C=C, C.tplbond.C], useful as insecticides, acaricides, and fungicides, were prepared Thus, chlorination of 4-ethynyl-1,3-dimethylpyrazole-5-carboxylic acid with SOCl2 followed by amidation with 2-(2-naphthoxy)-5-aminomethylpyridine gave 15% 4-ethynyl-1,3-dimethyl-N-[2-(2-naphthoxy)pyridin-5-ylmethyl]pyrazole-5-carboxamide (II). II showed fungicidal activity against Puccinia recondita at 250 ppm.
IT **243465-93-2P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolecarboxamides as insecticides, acaricides, and

L4 ANSWER 23 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
fungicides)
RN 243465-93-2 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 3-ethyl-1-methyl-N-[[6-(2-naphthalenyloxy)-3-pyridinyl]methyl]-4-(phenylethynyl)- (9CI) (CA INDEX NAME)

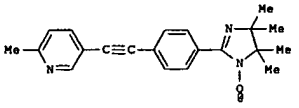


REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 24 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:511706 CAPLUS
DOCUMENT NUMBER: 131:242935
TITLE: Stable free imino and nitronyl nitroxyl radicals of the acetylene series: synthesis, electronic absorption spectra and magnetic resonance parameters
AUTHOR(S): Tretyakov, Eugene V.; Samoilova, Rimma I.; Ivanov, Yuri V.; Plyusnin, Victor F.; Pashchenko, Sergei V.; Vasilevsky, Sergei F.
CORPORATE SOURCE: Institute of Chemical Kinetics and Combustion, Siberian Branch of the Russian Academy of Sciences, Novosibirsk, 630090, Russia
SOURCE: Mendeleev Communications (1999), (3), 92-95
CODEN: MENCEX; ISSN: 0959-9436
PUBLISHER: Russian Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

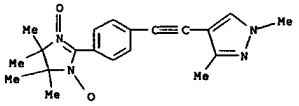


I

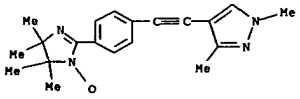


II

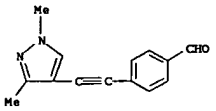
AB Methods for the synthesis of aryl(hetaryl)ethynylphenyl-2-imidazoline nitroxides (e.g. I) have been developed; the g-tensor and HFI components for imidazoline-1-oxyl were found to depend (in contrast to imidazoline-3-oxide-1-oxyl derivs., II) on the properties of substituent at the 2-position.
IT **220183-78-8P 220183-82-4P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(electronic absorption and ESR spectra of nitroxide radicals)
RN 220183-78-8 CAPLUS
CN 1H-Imidazol-1-yloxy, 2-[4-[(1,3-dimethyl-1H-pyrazol-4-yl)ethynyl]phenyl]-4,5-dihydro-4,4,5,5-tetramethyl-, 3-oxide (9CI) (CA INDEX NAME)



L4 ANSWER 24 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 220183-82-4 CAPLUS
CN 1H-Imidazol-1-yloxy, 2-[4-[(1,3-dimethyl-1H-pyrazol-4-yl)ethynyl]phenyl]-4,5-dihydro-4,4,5,5-tetramethyl- (9CI) (CA INDEX NAME)

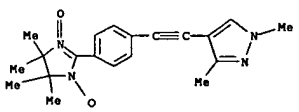


IT **220183-90-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate for preparation of nitroxides)
RN 220183-90-4 CAPLUS
CN Benzaldehyde, 4-[(1,3-dimethyl-1H-pyrazol-4-yl)ethynyl]- (9CI) (CA INDEX NAME)

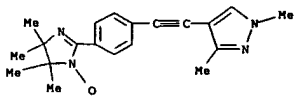


REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 25 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:803336 CAPLUS
DOCUMENT NUMBER: 130:153607
TITLE: A new family of stable 2-imidazoline nitroxides
AUTHOR(S): Vasilevsky, Sergey F.; Tretyakov, Eugene V.; Usov, Oleg M.; Molin, Yuri N.; Fokin, Sergei V.; Shwedenkov, Yuri G.; Ikorskii, Vladimir N.; Romanenko, Galina V.; Sagdeev, Renad Z.; Ovcharenko, Victor I.
CORPORATE SOURCE: Institute of Chemical Kinetics and Combustion, Siberian Branch of the Russian Academy of Sciences, Novosibirsk, 630090, Russia
SOURCE: Mendeleev Communications (1998), (6), 216-218
CODEN: MENCEX; ISSN: 0959-9436
PUBLISHER: Russian Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Methods of synthesizing stable 2-imidazoline nitroxides linked to a pyrazole moiety either directly or through a phenylethynyl bridge have been developed. An unusually strong temperature dependence of the effective magnetic moment for 2-(1-methylpyrazolyl-5)-4,4,5,5-tetramethyl-1-oxyl-2-imidazoline 3-oxide is observed
IT **220183-78-8P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and ESR)
RN 220183-78-8 CAPLUS
CN 1H-Imidazol-1-yloxy, 2-[4-[(1,3-dimethyl-1H-pyrazol-4-yl)ethynyl]phenyl]-4,5-dihydro-4,4,5,5-tetramethyl-, 3-oxide (9CI) (CA INDEX NAME)

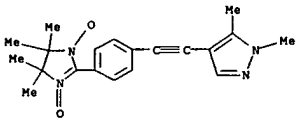


IT **220183-82-4P 220183-87-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 220183-82-4 CAPLUS
CN 1H-Imidazol-1-yloxy, 2-[4-[(1,3-dimethyl-1H-pyrazol-4-yl)ethynyl]phenyl]-4,5-dihydro-4,4,5,5-tetramethyl- (9CI) (CA INDEX NAME)



RN 220183-87-9 CAPLUS
CN 1H-Imidazol-1-yloxy, 2-[4-[(1,5-dimethyl-1H-pyrazol-4-yl)ethynyl]phenyl]-4,5-dihydro-4,4,5,5-tetramethyl-, 3-oxide (9CI) (CA INDEX NAME)

L4 ANSWER 25 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

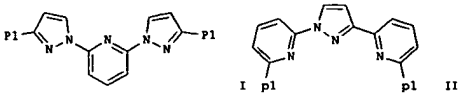


REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 26 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:374715 CAPLUS
DOCUMENT NUMBER: 126:350804
TITLE: Biospecific binding reactants labeled with luminescent lanthanide chelates and their use
INVENTOR(S): Rodriguez-Ubis, Juan Carlos; Takalo, Harri; Mukkala, Veli-matti
PATENT ASSIGNEE(S): Wallac Oy, Finland; Rodriguez-Ubis, Juan Carlos
SOURCE: Eur. Pat. Appl., 33 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 770610	A1	19970502	EP 1996-660056	19960909
R: DE, FR, GB				
US 5859215	A	19990112	US 1995-548174	19951025
PRIORITY APPLN. INFO.:			US 1995-548174 A	19951025
OTHER SOURCE(S):	MARPAT 126:350804			

GI

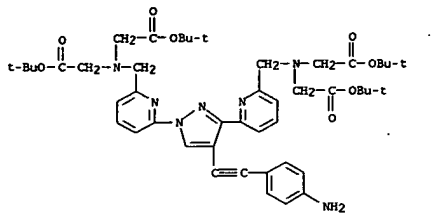


AB This invention relates to a detectable mol. comprising a biospecific binding reactant attached to a luminescent lanthanide chelate comprising a lanthanide ion and a chelating ligand (-O2CCH2)2NCH2-[A](-G1)-CH2N(CH2CO2-)(CH2CO2-) wherein -A- is a bivalent aromatic structure selected from pyridine-pyrazole compds. I, II, etc. and groups G1 or G2 are H, Cl, Br, I, CN, Ph, alkyl, alkoxy, etc., one of which is used for coupling the chelate to a biospecific binding reactant. The lanthanide ion is Eu(III), Tb(III), Dy(III) or Sm(III). The biospecific binding reactant may be selected from a group consisting of an antibody, antigen, receptor ligand, a specific binding protein, and a DNA or RNA probe.

IT **189805-29-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of luminescent lanthanide pyrazolediylbispyridinediyl and pyridinediylbispyrazolediyl bismethylenenitrilotetrakisacetato chelates for biospecific binding assays)

RN 189805-29-6 CAPLUS
CN Glycine, N,N'-[[4-[(4-aminophenyl)ethynyl]-1H-pyrazole-1,3-diyl]bis(6,2-pyridinediylmethylene)]bis[N-[2-(1,1-dimethylethoxy)-2-oxoethyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

L4 ANSWER 26 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

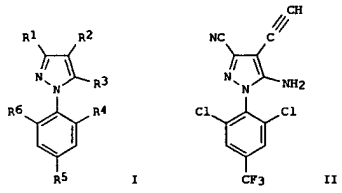


L4 ANSWER 27 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:257469 CAPLUS
DOCUMENT NUMBER: 126:238380
TITLE: Parasiticidal pyrazole derivatives and their preparation and use
INVENTOR(S): Banks, Bernard Joseph
PATENT ASSIGNEE(S): Pfizer Inc., USA; Pfizer Limited; Banks, Bernard Joseph
SOURCE: PCT Int. Appl., 93 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9707102	A1	19970227	WO 1996-EP3501	19960805
W: AU, BR, CA, CN, CZ, HU, IL, JP, KR, MX, NO, NZ, PL, RU, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
TW 381082	B	20000201	TW 1996-85108511	19960713
CA 2229173	AA	19970227	CA 1996-2229173	19960805
CA 2229173	C	20020702		
AU 9668712	A1	19970312	AU 1996-68712	19960805
AU 710736	B2	19990930		
CN 1192735	A	19980909	CN 1996-196207	19960805
JP 10510551	T2	19981013	JP 1997-508911	19960805
JP 3154413	B2	20010409		
EP 871617	A1	19981021	EP 1996-929222	19960805
EP 871617	B1	20011114		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
BR 9610608	A	19990217	BR 1996-10608	19960805
RU 2151766	C1	20000627	RU 1998-102359	19960805
AT 208762	E	20011115	AT 1996-929222	19960805
PT 871617	T	20020228	PT 1996-929222	19960805
ES 2165520	T3	20020316	ES 1996-929222	19960805
IL 122281	A1	20021110	IL 1996-122281	19960805
PL 185765	B1	20030731	PL 1996-324995	19960805
CZ 292275	B6	20030813	CZ 1998-392	19960805
ZA 9606758	A	19980209	ZA 1996-6758	19960808
NO 9800570	A	19980331	NO 1998-570	19980210
US 6255333	B1	20010703	US 1998-11815	19980211
PRIORITY APPLN. INFO.:			GB 1995-16454 A	19950811
			GB 1996-1128 A	19960119
			WO 1996-EP3501 W	19960805
OTHER SOURCE(S):	MARPAT 126:238380			

GI

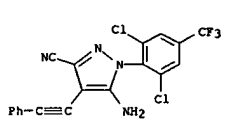
L4 ANSWER 27 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



AB Parasitical pyrazole derivs. I are disclosed [wherein: R1 = cyano, C1-6 alkoxycarbonyl, NO2, CHO, C1-6 alkanoyl, (halo)phenyl, (halo)alkyl; R2 = (un)substituted ethynyl, ethenyl, or 1-cyclohexenyl; R3 = H, C1-6 alkyl, halo, certain (un)substituted NH2, N-pyrrolyl, OH, C1-6 alkoxy, SH, (halo)alkyl(thio/sulfinyl/sulfonyl); R4, R5, R6 = H, halo, C1-6 (halo)alkyl, (halo)alkoxy, (halo)alkyl(thio/sulfinyl/sulfonyl), Ac, cyano, CONH2, CSNH2, OCF3, SCF3, SF5; and acceptable salts]. I are useful against arthropods, nematodes, helminths, and protozoa, and may also have antifeeding or repellent effects on insects. Approx. 90 examples were prepared For instance, 5-amino-3-cyano-1-(2,6-dichloro-4-trifluoromethylphenyl)pyrazole underwent iodination in the 4-position using N-iodosuccinimide, followed by Pd(PPh3)2Cl2-catalyzed coupling with HC.tplbond.CSiMe3 and desilylation using K2CO3 in MeOH, to give title compound II. In tests against the stable fly Stomoxys calcitrans, II gave 100% mortality at a dose of 0.005-100 μg per fly (direct application).

IT **188538-74-1P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of parasiticidal pyrazole derivs.)

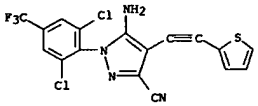
RN 188538-74-1 CAPLUS
CN 1H-Pyrazole-3-carbonitrile, 5-amino-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-4-(phenylethynyl)- (9CI) (CA INDEX NAME)



IT **188538-75-2P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of parasiticidal pyrazole derivs.)

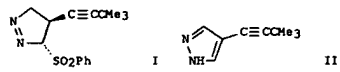
RN 188538-75-2 CAPLUS
CN 1H-Pyrazole-3-carbonitrile, 5-amino-1-[2,6-dichloro-4-

L4 ANSWER 27 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
(trifluoromethyl)phenyl]-4-(2-thienylethynyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 28 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN

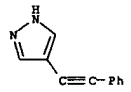
ACCESSION NUMBER: 1997:246220 CAPLUS
DOCUMENT NUMBER: 126:317341
TITLE: A convenient synthesis of alkynylpyrazoles
AUTHOR(S): Yoshimatsu, Mitsuhiro; Kawahigashi, Masataka; Honda, Eiji; Kataoka, Tadashi
CORPORATE SOURCE: Department of Chemistry, Faculty of Education, Gifu University, Gifu, 501-11, Japan
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1997), (5), 695-700
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:317341
GI



AB Diazomethane adds to enyne sulfones, e.g. Me3CC.tplbond.CCH:CHSO2Ph, regio- and stereoselectively to give 4-alkynyl-5-phenylsulfonyl-4,5-dihydro-3H-pyrazoles, e.g. I. These products are converted by MeLi into 4-alkynyl-1H-pyrazoles, e.g. II, in good yields. 4,5-Bis(alkynyl)-1H-pyrazoles are also obtained by the same procedure.

IT **82099-93-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of alkynylpyrazoles)

RN 82099-93-2 CAPLUS
CN 1H-Pyrazole, 4-(phenylethynyl)- (9CI) (CA INDEX NAME)



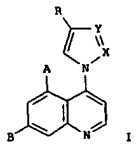
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 29 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:315238 CAPLUS
DOCUMENT NUMBER: 124:343296
TITLE: Preparation of azolylquinolines as agrochemical fungicides.
INVENTOR(S): Kurahashi, Yoshio; Moriya, Koichi; Sawada, Haruko; Sakuma, Haruhiko; Watanabe, Ryo; Ito, Asami
PATENT ASSIGNEE(S): Nihon Bayer Agrochem K.K., Japan
SOURCE: Eur. Pat. Appl., 52 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 703234	A1	19960327	EP 1995-114216	19950911
R: BE, CH, DE, ES, FR, GB, LI, NL				
JP 08143407	A2	19960604	JP 1995-97670	19950331
US 5622914	A	19970422	US 1995-529963	19950919
PRIORITY APPLN. INFO.:			JP 1994-251620 A	19940921
			JP 1995-97670 A	19950331

OTHER SOURCE(S): MARPAT 124:343296
GI

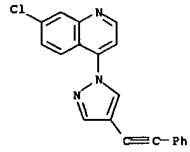


AB Title compds. [I; X = N, Y = CH; or Y = N, X = CH; R1 = halo, Ac, (substituted) alkyl, alkenyl, alkynyl, cycloalkyl; A = H, halo; B = halo, haloalkyl], were prepared Thus, 7-chloro-4-(4-iodo-1-pyrazolyl)quinoline in DMF was treated with CuI, (Ph3P)2PdCl2, and Me3SiC.tplbond.CH to give 7-chloro-4-(4-trimethylsilylethynyl-1-pyrazolyl)quinoline. The latter at 100 ppm gave 100% curative effect in barley infected with barley powdery mildew.

IT **176793-74-1P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azolylquinolines as agrochem. fungicides)

RN 176793-74-1 CAPLUS
CN Quinoline, 7-chloro-4-[4-(phenylethynyl)-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)

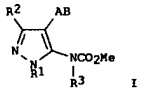
L4 ANSWER 29 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L4 ANSWER 30 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:735491 CAPLUS
DOCUMENT NUMBER: 123:169617
TITLE: Preparation of methyl N-pyrazolylcarbamate agricultural-horticultural fungicides
INVENTOR(S): Oda, Masatsugu; Katsurada, Manabu; Tomita, Hirofumi
PATENT ASSIGNEE(S): Mitsubishi Chemical Corp., Japan
SOURCE: Eur. Pat. Appl., 23 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 658547	A1	19950621	EP 1994-119428	19941208
EP 658547	B1	19980311		
R: BE, CH, DE, DK, ES, FR, GB, IT, LI, NL				
JP 07258219	A2	19951009	JP 1994-299655	19941202
PRIORITY APPLN. INFO.:			JP 1993-313520 A	19931214

OTHER SOURCE(S): MARPAT 123:169617
GI



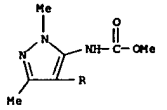
I

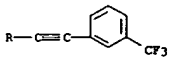
AB The title compds. [I; A = O, CO, OCH2, CH2O, CH2S, C.tplbond.C, CH:CH, CH2CH2, etc.; B = H, (un)substituted aryl, (un)substituted heterocyclyl; R1, R2 = H, C1-4 alkyl; R3 = R1, C2-5 alkynyl, alkylthioalkyl, alkoxyalkyl], useful as agricultural and horticultural fungicides, are prepared and I-containing formulations presented. Thus, I (A = OCH2, B = Ph, R1 = R2 = Me, R3 = CH2C.tplbond.CH), a viscous liquid, was prepared and demonstrated a 100% cure of Erysiphe graminis-infected wheat at an application concentration of 200 ppm.

IT **166315-75-9P**
RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of Me N-pyrazolylcarbamate agricultural-horticultural fungicides)

RN 166315-75-9 CAPLUS
CN Carbamic acid, [1,3-dimethyl-4-[[3-(trifluoromethyl)phenyl]ethynyl]-1H-pyrazol-5-yl]-, methyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 30 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

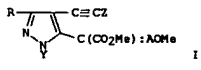




L4 ANSWER 31 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1994:164166 CAPLUS
DOCUMENT NUMBER: 120:164166
TITLE: Preparation of pyrazoles as agrochemical fungicides
INVENTOR(S): Eberle, Martin; Schaub, Fritz
PATENT ASSIGNEE(S): Sandoz Ltd., Switz.; Sandoz-Patent-GmbH; Sandoz-Erfindungen Verwaltungsgesellschaft M.B.H.
SOURCE: Eur. Pat. Appl., 15 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 571326	A1	19931124	EP 1993-810324	19930504
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
HU 64180	A2	19931228	HU 1993-1248	19930429
CA 2095941	AA	19931114	CA 1993-2095941	19930511
AU 9338485	A1	19931118	AU 1993-38485	19930511
AU 666717	B2	19960222		
IL 105668	A1	19970318	IL 1993-105668	19930511
CZ 282767	B6	19971015	CZ 1993-864	19930511
BR 9301823	A	19931116	BR 1993-1823	19930512
JP 06032781	A2	19940208	JP 1993-110313	19930512
RU 2098410	C1	19971210	RU 1993-5298	19930512
US 5300521	A	19940405	US 1993-116234	19930901
PRIORITY APPLN. INFO.:			GB 1992-10224 A	19920513
			GB 1993-4198 A	19930302
			US 1993-60769 B1	19930510

OTHER SOURCE(S): MARPAT 120:164166
GI



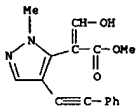
I

AB Title compds. I (R = H, C1-4 alkyl, (substituted) aryl, F3C; Y = C1-4 alkyl, (substituted) aryl; A = N, HC; Z = (substituted) hydrocarbyl, (substituted) heterocyclyl). To Me α-(1-methyl-4-phenylthinyl-5-pyrazol)-β-hydroxyacrylate (preparation given) was added MeI and the mixture stirred for 3 h at 25° to give E + Z-I (R = H, Y = Me, A = HC, Z = Ph). A similar prepared compound E-I (R = Y = Me, A = HC, Z = 4-ClC6H4) showed >90% control of Sphaerotheca fuliginea on cucumber. Addnl. I were prepared and evaluated as agrochem. fungicides.

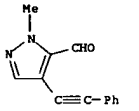
IT **153208-20-9P 153208-22-1P 153208-23-2P**
153208-24-3P 153208-25-4P 153208-28-7P
153208-29-8P 153208-30-1P 153208-31-2P
153208-32-3P 153208-34-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of agrochem. fungicides)

RN 153208-20-9 CAPLUS
CN 1H-Pyrazole-5-acetic acid, α-(hydroxymethylene)-1-methyl-4-(phenylethynyl)-, methyl ester (9CI) (CA INDEX NAME)

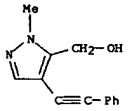
L4 ANSWER 31 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



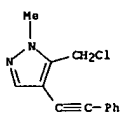
RN 153208-22-1 CAPLUS
CN 1H-Pyrazole-5-carboxaldehyde, 1-methyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)



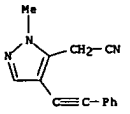
RN 153208-23-2 CAPLUS
CN 1H-Pyrazole-5-methanol, 1-methyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)



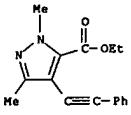
RN 153208-24-3 CAPLUS
CN 1H-Pyrazole, 5-(chloromethyl)-1-methyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)



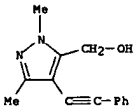
RN 153208-25-4 CAPLUS
CN 1H-Pyrazole-5-acetonitrile, 1-methyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)



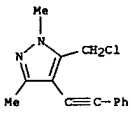
RN 153208-28-7 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 1,3-dimethyl-4-(phenylethynyl)-, ethyl ester (9CI) (CA INDEX NAME)



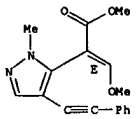
RN 153208-29-8 CAPLUS
CN 1H-Pyrazole-5-methanol, 1,3-dimethyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)



RN 153208-30-1 CAPLUS
CN 1H-Pyrazole, 5-(chloromethyl)-1,3-dimethyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)

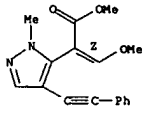


RN 153208-31-2 CAPLUS
CN 1H-Pyrazole-5-acetonitrile, 1,3-dimethyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)



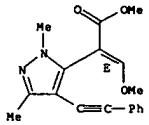
RN 153208-01-6 CAPLUS
CN 1H-Pyrazole-5-acetic acid, α-(methoxymethylene)-1-methyl-4-(phenylethynyl)-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



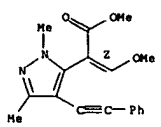
RN 153208-02-7 CAPLUS
CN 1H-Pyrazole-5-acetic acid, α-(methoxymethylene)-1,3-dimethyl-4-(phenylethynyl)-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

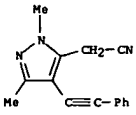
Double bond geometry as shown.



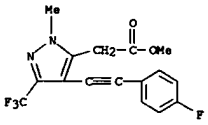
RN 153208-03-8 CAPLUS
CN 1H-Pyrazole-5-acetic acid, α-(methoxymethylene)-1,3-dimethyl-4-(phenylethynyl)-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

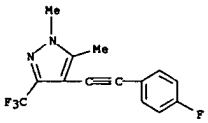




RN 153208-32-3 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[(4-fluorophenyl)ethynyl]-1-methyl-3-(trifluoromethyl)-, methyl ester (9CI) (CA INDEX NAME)



RN 153208-34-5 CAPLUS
CN 1H-Pyrazole, 4-[(4-fluorophenyl)ethynyl]-1,5-dimethyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

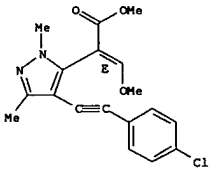


IT **153208-00-5P 153208-01-6P 153208-02-7P 153208-03-8P 153208-04-9P 153208-05-0P 153208-06-1P 153208-07-2P 153208-09-4P 153208-10-7P 153208-11-8P 153208-12-9P 153208-13-0P 153208-14-1P 153208-15-2P 153208-16-3P 153208-17-4P 153208-18-5P 153208-19-6P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as agrochem. fungicide)
RN 153208-00-5 CAPLUS
CN 1H-Pyrazole-5-acetic acid, α-(methoxymethylene)-1-methyl-4-(phenylethynyl)-, methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

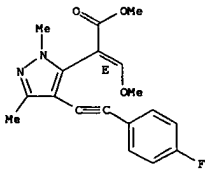
RN 153208-04-9 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[(4-chlorophenyl)ethynyl]-α-(methoxymethylene)-1,3-dimethyl-, methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



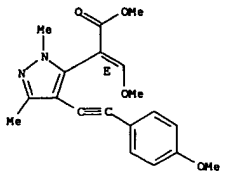
RN 153208-05-0 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[(4-fluorophenyl)ethynyl]-α-(methoxymethylene)-1,3-dimethyl-, methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



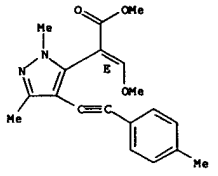
RN 153208-06-1 CAPLUS
CN 1H-Pyrazole-5-acetic acid, α-(methoxymethylene)-4-[(4-methoxyphenyl)ethynyl]-1,3-dimethyl-, methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



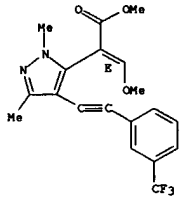
RN 153208-07-2 CAPLUS
CN 1H-Pyrazole-5-acetic acid, α-(methoxymethylene)-1,3-dimethyl-4-[(4-methylphenyl)ethynyl]-, methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

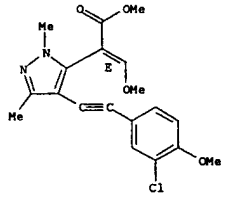


RN 153208-09-4 CAPLUS
CN 1H-Pyrazole-5-acetic acid, α-(methoxymethylene)-1,3-dimethyl-4-[[3-(trifluoromethyl)phenyl]ethynyl]-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

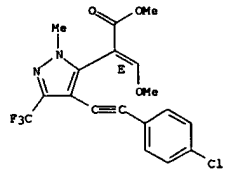


RN 153208-10-7 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[(3,4-dichlorophenyl)ethynyl]-α-



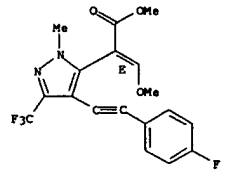
RN 153208-13-0 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[(4-chlorophenyl)ethynyl]-α-(methoxymethylene)-1-methyl-3-(trifluoromethyl)-, methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 153208-14-1 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[(4-fluorophenyl)ethynyl]-α-(methoxymethylene)-1-methyl-3-(trifluoromethyl)-, methyl ester, (E)- (9CI) (CA INDEX NAME)

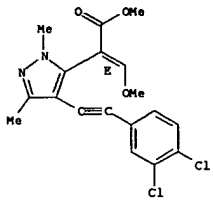
Double bond geometry as shown.



RN 153208-15-2 CAPLUS

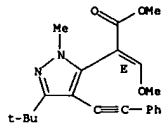
(methoxymethylene)-1,3-dimethyl-, methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 153208-11-8 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 3-(1,1-dimethylethyl)-α-(methoxymethylene)-1-methyl-4-(phenylethynyl)-, methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

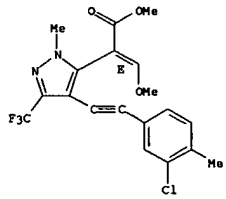


RN 153208-12-9 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[(3-chloro-4-methoxyphenyl)ethynyl]-α-(methoxymethylene)-1,3-dimethyl-, methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

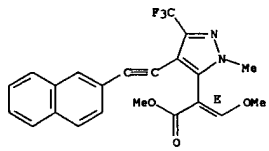
CN 1H-Pyrazole-5-acetic acid, 4-[(3-chloro-4-methylphenyl)ethynyl]-α-(methoxymethylene)-1-methyl-3-(trifluoromethyl)-, methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 153208-16-3 CAPLUS
CN 1H-Pyrazole-5-acetic acid, α-(methoxymethylene)-1-methyl-4-(2-naphthalenylethynyl)-3-(trifluoromethyl)-, methyl ester, (E)- (9CI) (CA INDEX NAME)

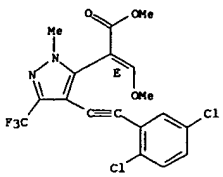
Double bond geometry as shown.



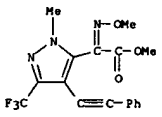
RN 153208-17-4 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[(2,5-dichlorophenyl)ethynyl]-α-(methoxymethylene)-1-methyl-3-(trifluoromethyl)-, methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

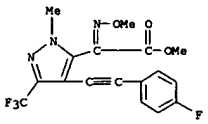
L4 ANSWER 31 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



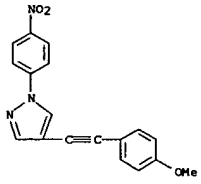
RN 153208-18-5 CAPLUS
CN 1H-Pyrazole-5-acetic acid, α-(methoxyimino)-1-methyl-4-(phenylethynyl)-3-(trifluoromethyl)-, methyl ester (9CI) (CA INDEX NAME)



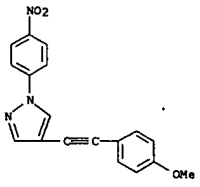
RN 153208-19-6 CAPLUS
CN 1H-Pyrazole-5-acetic acid, 4-[(4-fluorophenyl)ethynyl]-α-(methoxyimino)-1-methyl-3-(trifluoromethyl)-, methyl ester (9CI) (CA INDEX NAME)



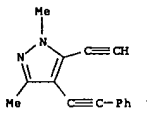
L4 ANSWER 32 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1994:134362 CAPLUS
DOCUMENT NUMBER: 120:134362
TITLE: The synthesis of electron donor-acceptor substituted pyrazoles
AUTHOR(S): Miller, R. D.; Reiser, O.
CORPORATE SOURCE: Almaden Res. Cent., IBM Res. Div., San Jose, CA, 95120-6099, USA
SOURCE: Journal of Heterocyclic Chemistry (1993), 30(3), 755-63
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 120:134362
AB A variety of 1,3-and 1,5-donor-acceptor substituted pyrazole derivs. have been synthesized by the cyclocondensation of α,β-ethynyl ketones with substituted phenylhydrazines. The regioselectivity of the cyclization depends on the reaction conditions in a manner consistent with competitive 1,2- and 1,4-addition followed by ring closure. 1,4-Disubstituted derivs. can be prepared from the corresponding 4-iodopyrazole using palladium catalyzed carbon-carbon bond forming reactions. The pyrazole chromophores are expected to show interesting nonlinear optical properties.
IT 148508-13-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 148508-13-8 CAPLUS
CN 1H-Pyrazole, 4-[(4-methoxyphenyl)ethynyl]-1-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



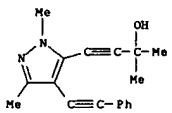
L4 ANSWER 33 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1993:448851 CAPLUS
DOCUMENT NUMBER: 119:48851
TITLE: Heterocyclic azole nonlinear optical chromophores. 1. Donor-acceptor substituted pyrazole derivatives
AUTHOR(S): Miller, Robert D.; Moylan, Christopher R.; Reiser, Oliver; Walsh, Cecilia A.
CORPORATE SOURCE: Almaden Res. Cent., IBM Res., San Jose, CA, 95120-6099, USA
SOURCE: Chemistry of Materials (1993), 5(5), 625-32
CODEN: CMATEX; ISSN: 0897-4756
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The synthesis of a variety of 1,3, 1,4, and 1,5 donor-acceptor conjugation-extended substituted pyrazole derivs. was described; their spectroscopic and nonlinear optical properties were studied. These materials are thermally stable and absorb strongly in the UV-visible region, albeit at much shorter wavelengths than comparably substituted cyclic azapolyenes such as 2-pyrazolines. Quadratic hyperpolarizability measurements suggest that the pyrazoles are significantly nonlinear, and that 1,3 and 1,4 substitution is preferred. 1,5 Substitution causes a significant drop in the nonlinearity and a blue shift in the long-wavelength absorption maximum, presumably due to a twisting and partial deconjugation of the substituents to relieve unfavorable steric interactions. The exptl. results are compared with those predicted by simple finite field computational procedures.
IT 148508-13-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and nonlinear optical property of)
RN 148508-13-8 CAPLUS
CN 1H-Pyrazole, 4-[(4-methoxyphenyl)ethynyl]-1-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 34 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1992:550470 CAPLUS
DOCUMENT NUMBER: 117:150470
TITLE: Equilibrium carbon acidity of acetylenic derivatives of N-alkyl azoles in DMSO
AUTHOR(S): Belov, A. I.; Terekhova, M. I.; Petrov, E. S.; Vasilevskii, S. F.; Shvartsberg, M. S.
CORPORATE SOURCE: L. Ya. Karpov Sci.-Res. Phys.-Chem. Inst., Moscow, 103064, Russia
SOURCE: Izvestiya Akademi Nauk, Seriya Khimicheskaya (1992), (3), 507-12
CODEN: IASKEA; ISSN: 0002-3353
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB The CH acidity of alkynyl azoles I increased with X = NH in the series γ < δ < β (with remaining X = CH). For fixed disposition of NH in the ring, α-ethynyl azoles had a higher CH acidity than β-ethynyl azoles. CH acidity was also increased by increasing the number of N atoms in the heterocycle; thus, ethynyltetrazole had the lowest pK of all compds. examined The CH acidity of butadiynylpyrazole II (pK = 24-26) was 5-7 orders of magnitude greater than that of the corresponding ethynyl derivative
IT 94990-01-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and carbon acidity of)
RN 94990-01-9 CAPLUS
CN 1H-Pyrazole, 5-ethynyl-1,3-dimethyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)

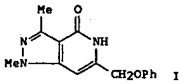


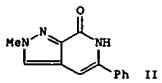
IT 94990-05-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and fragmentation of, to alkynylpyrazole derivative)
RN 94990-05-3 CAPLUS
CN 3-Butyn-2-ol, 4-[1,3-dimethyl-4-(phenylethynyl)-1H-pyrazol-5-yl]-2-methyl- (9CI) (CA INDEX NAME)

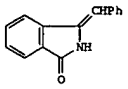


L4 ANSWER 35 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1991:164091 CAPLUS
DOCUMENT NUMBER: 114:164091
TITLE: Cyclization of vicinal acetylenic amides of pyrazolecarboxylic and benzoic acids
AUTHOR(S): Vasilevskii, S. F.; Shvartsberg, M. S.
CORPORATE SOURCE: Inst. Khim. Kinet. Goren., Novosibirsk, USSR
SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1990), (9), 2089-93
CODEN: IASKA6; ISSN: 0002-3353
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 114:164091
GI


I

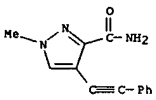

II


III

AB The title reaction of acetylenic amides, e.g., o-H2NCOC6H4C.tplbond.CPh, in presence of KOH gives 5-, or 6-membered lactams, e.g., derivs. of pyrazolopyridinones (I) and (II) and isoindolone (III), in 70-85% yield. The condensation of iodopyrazolecarboxamides with CuC.tplbond.CPh (IV) gives the corresponding pyrazolylacetylenes and is not accompanied by intramol. cyclization of these products. Literature data concerning cyclocondensation of o-IC6H4CONH2 with (IV) to give 3-amino-2-phenylindenone could not be reproduced.

IT **133053-59-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and intramol. cyclization of)

RN 133053-59-5 CAPLUS
CN 1H-Pyrazole-3-carboxamide, 1-methyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 35 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

L4 ANSWER 36 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN

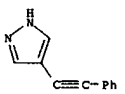
ACCESSION NUMBER: 1988:510317 CAPLUS
DOCUMENT NUMBER: 109:110317
TITLE: Pyrazoles II. The chemistry of pyrazolylalkynes
AUTHOR(S): Heinisch, Gottfried; Holzer, Wolfgang; Obala, Claudia
CORPORATE SOURCE: Inst. Pharm. Chem., Univ. Wien, Vienna, A-1090, Austria
SOURCE: Monatshefte fuer Chemie (1988), 119(2), 253-62
CODEN: MOCMB7; ISSN: 0026-9247
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 109:110317
GI


I

AB Ethynylation of N-protected pyrazoles I (R = Bz, tosyl; R1 = Br, iodo) with HC.tplbond.CR2 (R2 = Ph, CMe2OH, SiMe3) in the presence of catalysts (Ph3P)2PdCl2-CuI in Et3N solution gave ethynylpyrazoles I (R = Bz, tosyl; R1 = C.tplbond.CR2). Deprotection with MeOH gave I (R = H, R1 = C.tplbond.CPh, C.tplbond.CCMe2OH). HgO mediated hydration of I (R = H, R1 = C.tplbond.CPh, C.tplbond.CH) gave ketones I (R = H, R1 = Ac, PhCH2CO).

IT **82099-93-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and mercuric oxide mediated dehydration of)

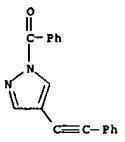
RN 82099-93-2 CAPLUS
CN 1H-Pyrazole, 4-(phenylethynyl)- (9CI) (CA INDEX NAME)



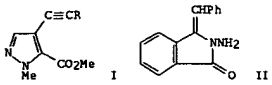
IT **116228-42-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and methanolic deprotection of)

RN 116228-42-3 CAPLUS
CN 1H-Pyrazole, 1-benzoyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)

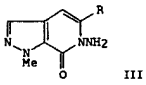
L4 ANSWER 36 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

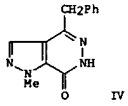


L4 ANSWER 37 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1988:37758 CAPLUS
DOCUMENT NUMBER: 108:37758
TITLE: Synthesis and heterocyclization of acetylene derivatives of phenyl- and pyrazolylcarboxylic acid hydrazides
AUTHOR(S): Pozdnyakov, A. V.
CORPORATE SOURCE: Novosib. Gos. Univ., Novosibirsk, USSR
SOURCE: Mater. Vses. Nauchn. Stud. Konf. "Stud. Nauchno-Tekh. Prog.": Khim., 22nd (1984), 26-30. Editor(s): Rait, V. K. Novosib. Gos. Univ.: Novosibirsk, USSR.
CODEN: 55LIA9
DOCUMENT TYPE: Conference
LANGUAGE: Russian
GI

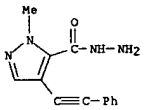

I

II


III

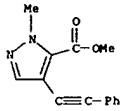

IV

AB Reaction of appropriate iodo compds. with RC.tplbond.CH in the presence of Pd(PPh3)2Cl2-CuI gave 2-RC:tplbond.CC6H4CO2Me (R = Ph, PhOCH2, HOCMe2) and pyrazolecarboxylates I (R = Ph, PhOCH2, morpholinomethyl). These on hydrazinolysis and ring closure with alkali gave methylenephthalimide II or pyrazolopyridines III. Cyclization with Cu(I) in DMF gave pyridazines such as IV.
IT **87612-14-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)
RN 87612-14-4 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 1-methyl-4-(phenylethynyl)-, hydrazide (9CI) (CA INDEX NAME)



IT **79229-75-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

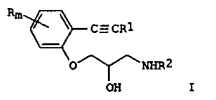
L4 ANSWER 37 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
(Reactant or reagent)
(prepn. and hydrazinolysis of)
RN 79229-75-7 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 1-methyl-4-(phenylethynyl)-, methyl ester (9CI) (CA INDEX NAME)

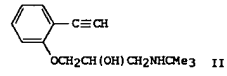


L4 ANSWER 38 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1987:477423 CAPLUS
DOCUMENT NUMBER: 107:77423
TITLE: Preparation of heteroaromatic acetylenes useful as antihypertensive agents
INVENTOR(S): Carson, John R.
PATENT ASSIGNEE(S): McNeilab, Inc., USA
SOURCE: U.S., 8 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4663334	A	19870505	US 1985-807551	19851211
US 4728666	A	19880301	US 1986-934371	19861124
CA 1292739	A1	19911203	CA 1986-524856	19861209
DK 8605946	A	19870612	DK 1986-5946	19861210
FI 8605028	A	19870612	FI 1986-5028	19861210
NO 8604987	A	19870612	NO 1986-4987	19861210
EP 226447	A2	19870624	EP 1986-309601	19861210
EP 226447	A3	19880831		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 62175460	A2	19870801	JP 1986-292673	19861210
ZA 8609333	A	19880727	ZA 1986-9333	19861210
CN 86108922	A	19870805	CN 1986-108922	19861211
HU 44013	A2	19880128	HU 1986-5174	19861211
HU 196373	B	19881128		
AU 8666424	A1	19880616	AU 1986-66424	19861211
AU 597319	B2	19900531		

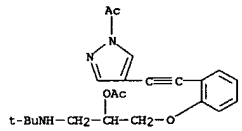
PRIORITY APPLN. INFO.: US 1985-807551 A3 19851211
OTHER SOURCE(S): CASREACT 107:77423
GI


I

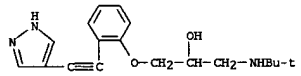

II

AB Title compds. I [R = alkyl, alkoxy, halo, alkoxyalkyl, carboxamidoalkyl, Cl, F, Br; m = 0-2; R1 = (un)substituted heterocycyl; R2 = C3-7 alkyl], useful as antihypertensives, are prepared A THF/Et3N solution of 6.1 g ethynylphenoxypropanolamine II was coupled with 5.8 g 4-bromopyridine in the presence of 0.14 g (Ph3P)4Pd and 0.05 g CuI over 18 h under a N atmospheric
to give I (m = 0, R1 = 4-pyridinyl, R2 = CMe3), isolated as the fumarate salt. This compound at 30 mg/kg orally caused a 46 mm Hg drop in blood pressure (sustained for 7.5 h) in standard spontaneously hypertensive rat testing.
IT **109684-43-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deacetylation of)
RN 109684-43-7 CAPLUS

L4 ANSWER 38 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN 1H-Pyrazole, 1-acetyl-4-[[2-[2-(acetyloxy)-3-[(1,1-dimethylethyl)amino]propoxy]phenyl]ethynyl]- (9CI) (CA INDEX NAME)



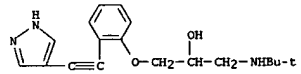
IT **109684-28-8P 109684-39-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as antihypertensive)
RN 109684-28-8 CAPLUS
CN 2-Propanol, 1-[(1,1-dimethylethyl)amino]-3-[2-(1H-pyrazol-4-ylethynyl)phenoxy]- (9CI) (CA INDEX NAME)



RN 109684-39-1 CAPLUS
CN 2-Propanol, 1-[(1,1-dimethylethyl)amino]-3-[2-(1H-pyrazol-4-ylethynyl)phenoxy]-, (2E)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 109684-28-8
CMF C18 H23 N3 O2

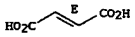


CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

L4 ANSWER 38 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



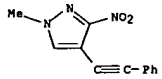
L4 ANSWER 39 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1987:176241 CAPLUS
DOCUMENT NUMBER: 106:176241
TITLE: Synthesis of nitropyrazolylacetylenes and attempts at their cyclization
AUTHOR(S): Vasilevskii, S. F.
CORPORATE SOURCE: Inst. Khim. Kinet. Goren., Novosbirsk, USSR
SOURCE: Izvestiya Sibirskogo Otdeleniya Akademii Nauk SSSR, Seriya Khimicheskikh Nauk (1986), (4), 105-7
CODEN: IZSKAB; ISSN: 0002-3426
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 106:176241

AB 4-Iodo-1-methyl-3-nitropyrazole was condensed with CuC.tplbond.CPh in pyridine 1.5 h at 115° to give 94% 1-methyl-3-nitro-4-(phenylethynyl)pyrazole. Analogously, 5-iodo-1,3-dimethyl-4-nitropyrazole gave 83.1% 5-phenylethynyl derivative and condensation with Ph.tplbond.CH in Et2NH containing Cu and (Ph3P)2PdCl2 gave 70% 1,3-dimethyl-4-nitropyrazole.

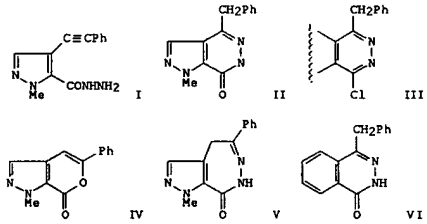
IT **107879-57-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 107879-57-2 CAPLUS
CN 1H-Pyrazole, 1-methyl-3-nitro-4-(phenylethynyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 40 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN

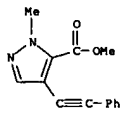
ACCESSION NUMBER: 1986:34057 CAPLUS
DOCUMENT NUMBER: 104:34057
TITLE: Cyclization of hydrazides of vicinal phenylethynyl derivatives of N-methylpyrazole-5-carboxylic and benzoic acids
AUTHOR(S): Vasilevskii, S. F.; Pozdnyakov, A. V.; Shvartsberg, M. S.
CORPORATE SOURCE: Inst. Khim. Kinet. Goren., Novosibirsk, USSR
SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1985), (6), 1367-70
CODEN: IASKA6; ISSN: 0002-3353
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 104:34057
GI



AB Treating hydrazide I with CuCl in DMF gave 70.6% pyrazolopyridazine II which was chlorinated by POCl3 to give 59.3% III. Treating pyranopyrazole IV with N2H4.H2O gave 59.6% pyrazolodiazepinone V. Analogously obtained were the corresponding derivs. from (phenylethynyl) benzoic acid, e.g., benzopyridazinone VI.

IT **79229-75-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and condensation with hydrazine hydrate)

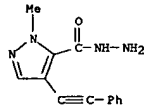
RN 79229-75-7 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 1-methyl-4-(phenylethynyl)-, methyl ester (9CI) (CA INDEX NAME)



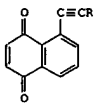
L4 ANSWER 40 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

IT **87612-14-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization reactions of)

RN 87612-14-4 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 1-methyl-4-(phenylethynyl)-, hydrazide (9CI) (CA INDEX NAME)

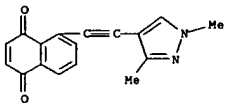


L4 ANSWER 41 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1985:95365 CAPLUS
DOCUMENT NUMBER: 102:95365
TITLE: 5-(Arylethynyl)-1,4-naphthoquinones
AUTHOR(S): Ivashkina, N. V.; Romanov, V. S.; Moroz, A. A.; Shvartsberg, M. S.
CORPORATE SOURCE: Inst. Khim. Kinet. Goren., Novosibirsk, USSR
SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1984), (11), 2561-5
CODEN: IASKA6; ISSN: 0002-3353
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 102:95365
GI

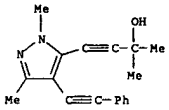


I

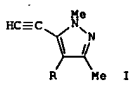
AB The title compds. [I; R = (un)substituted Ph, 2-naphthyl, 1,3-dimethyl-1H-pyrazol-4-yl] were prepared in 44-75.5% yield from 5-iodo-1,4-naphthoquinone and Cu acetylides.
IT **94849-13-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 94849-13-5 CAPLUS
CN 1,4-Naphthalenedione, 5-[(1,3-dimethyl-1H-pyrazol-4-yl)ethynyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 42 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

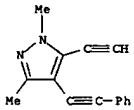


L4 ANSWER 42 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1985:95162 CAPLUS
DOCUMENT NUMBER: 102:95162
TITLE: Synthesis and study of CH-acidity of some ethynylazoles
AUTHOR(S): Belov, A. I.
CORPORATE SOURCE: Novosib. Gos. Univ., Novosibirsk, USSR
SOURCE: Mater. Vses. Nauchn. Stud. Konf. "Stud. Nauchno-Tekh. Prog.": Khim., 21st (1983), 9-13. Editor(s): Likanskaya, L. D. Novosib. Gos. Univ.: Novosibirsk, USSR.
CODEN: 52TOAC
DOCUMENT TYPE: Conference
LANGUAGE: Russian
GI



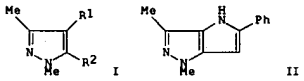
I

AB A linear correlation was observed between pK values of ethynylpyrazoles I (R = H, NH2, PhC.tplbond.C, Cl, Br, I) and substituent consts. σ. The results indicate no conjugation between the ethynyl and the π-electron ring systems. The preparation of ethynylpyrazoles is described.
IT **94990-01-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and CH-acidity of, substituent effect in)
RN 94990-01-9 CAPLUS
CN 1H-Pyrazole, 5-ethynyl-1,3-dimethyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)



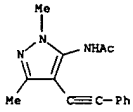
IT **94990-05-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and elimination reaction of)
RN 94990-05-3 CAPLUS
CN 3-Butyn-2-ol, 4-[1,3-dimethyl-4-(phenylethynyl)-1H-pyrazol-5-yl]-2-methyl- (9CI) (CA INDEX NAME)

L4 ANSWER 43 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1983:198102 CAPLUS
DOCUMENT NUMBER: 98:198102
TITLE: Cyclization of vicinal acetylenylaminopyrazoles
AUTHOR(S): Vasilevskii, S. F.; Anisimova, T. V.; Shvartsberg, M. S.
CORPORATE SOURCE: Inst. Khim. Kinet. Goren., Novosibirsk, USSR
SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1983), (3), 688-90
CODEN: IASKA6; ISSN: 0002-3353
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 98:198102
GI



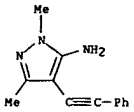
I II

AB Iodination of pyrazole I (R = R1 = H) by iodine-BuLi gave 60% I (R = iodo, R1 = H), which was nitrated to give 80.5% I (R = iodo, R1 = NO2), which was reduced by SnCl2 to give 53% I (R = iodo, R1 = NH2). The latter was ethynylated by CuC.tplbond.CPh to give 82% I (R = C.tplbond.CPh, R1 = NH2), which was cyclized in the presence of CuI-CuC.tplbond.CPh in DMF to give 65% II.
IT **85779-97-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 85779-97-1 CAPLUS
CN Acetamide, N-[1,3-dimethyl-4-(phenylethynyl)-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)



IT **85779-95-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 85779-95-9 CAPLUS
CN 1H-Pyrazol-5-amine, 1,3-dimethyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 43 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L4 ANSWER 44 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN

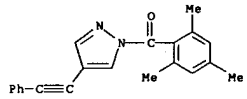
ACCESSION NUMBER: 1982:406216 CAPLUS
DOCUMENT NUMBER: 97:6216
TITLE: Synthetic inhibitors of alcohol dehydrogenase. Pyrazoles containing an unsaturated hydrocarbon residue in the 4-position
AUTHOR(S): Tolf, Bo Ragnar; Dahlbom, Richard; Theorell, Hugo; Aakeson, Aake
CORPORATE SOURCE: Biomed. Cent., Univ. Uppsala, Uppsala, S-751 23, Swed.
SOURCE: Acta Chemica Scandinavica, Series B: Organic Chemistry and Biochemistry (1982), B36(2), 101-7
CODEN: ACBOCV; ISSN: 0302-4369
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

I

AB Fourteen pyrazoles I (R = C.tplbond.CH, C.tplbond.CBu, C.tplbond.CPh, CH:CH2, PhC:CH, CH2Ph, (CH2)3C.tplbond.CH, etc.; R1 = H) were prepared from I (R = iodo, R1 = 2,4,6-Me3C6H2) via I (R = CH2OH, C.tplbond.CBu, C.tplbond.CPh, R1 = 2,4,6-Me3C6H2) or from I [R = Br, R1 = H; R = HO(CH2)3, R1 = H]. I were tested for ability to inhibit the enzyme alc. dehydrogenase and were less active than the corresponding saturated analogs.

IT **82100-18-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenation of)

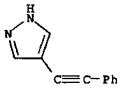
RN 82100-18-3 CAPLUS
CN 1H-Pyrazole, 4-(phenylethynyl)-1-(2,4,6-trimethylbenzoyl)- (9CI) (CA INDEX NAME)



IT **82099-93-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and inhibition of alc. dehydrogenase by)

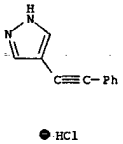
RN 82099-93-2 CAPLUS
CN 1H-Pyrazole, 4-(phenylethynyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 44 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



IT **82100-15-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

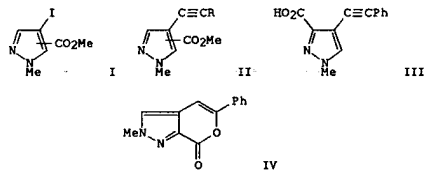
RN 82100-15-0 CAPLUS
CN 1H-Pyrazole, 4-(phenylethynyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L4 ANSWER 45 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1981:550523 CAPLUS
DOCUMENT NUMBER: 95:150523
TITLE: Cyclization of acetylenylpyrazolecarboxylic acids
AUTHOR(S): Shvartsberg, M. S.; Vasilevskii, S. F.; Anisimova, T. V.; Gerasimov, V. A.
CORPORATE SOURCE: Inst. Khim. Kinet. Goreniya, Novosibirsk, USSR
SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1981), (6), 1342-8
CODEN: IASKA6; ISSN: 0002-3353
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 95:150523
GI

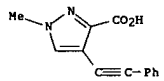


I II III IV

AB Acetylenyl-N-methylpyrazolecarboxylic esters containing acetylenyl substituents and ester groups on neighboring atoms, e.g., I (substituted in 3 or 5 position, and HC.tplbond.CR (R = CH2OMe, morpholinomethyl, Ph, CPhMeOH) gave the products of iodine substitution II. With a similar acid, e.g., III, and PhC.tplbond.CCu, pyranopyrazole IV was obtained.

IT **79229-57-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of, with phenylethynylcopper)

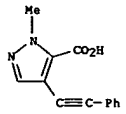
RN 79229-57-5 CAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 1-methyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)



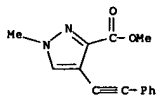
IT **79229-67-7P 79229-73-5P 79229-75-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 79229-67-7 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 1-methyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)

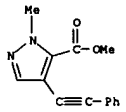
L4 ANSWER 45 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



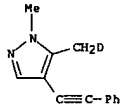
RN 79229-73-5 CAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 1-methyl-4-(phenylethynyl)-, methyl ester (9CI) (CA INDEX NAME)



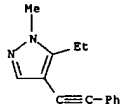
RN 79229-75-7 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 1-methyl-4-(phenylethynyl)-, methyl ester (9CI) (CA INDEX NAME)



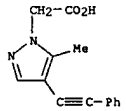
L4 ANSWER 46 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



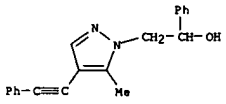
RN 71443-56-6 CAPLUS
CN 1H-Pyrazole, 5-ethyl-1-methyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)



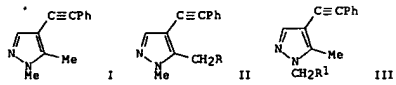
RN 71443-57-7 CAPLUS
CN 1H-Pyrazole-1-acetic acid, 5-methyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)



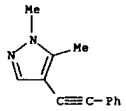
RN 71443-58-8 CAPLUS
CN 1H-Pyrazole-1-ethanol, 5-methyl-α-phenyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 46 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1979:540770 CAPLUS
DOCUMENT NUMBER: 91:140770
TITLE: Acidity of methyl substituents in a pyrazole ring
AUTHOR(S): Sinyakov, A. N.; Shvartsberg, M. S.
CORPORATE SOURCE: Inst. Khim. Kinet. Goreniya, Novosibirsk, USSR
SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1979), (5), 1126-8
CODEN: IASKA6; ISSN: 0002-3353
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI

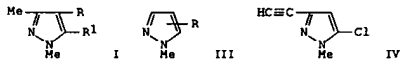


AB Treatment of the dimethylpyrazole I with NaNH2 in NH3(l) and then with D2O or MeI gave pyrazoles II (R = D, ICH2; resp.), whereas treatment of I with BuLi in Et2O and then with CO2 or B2H gave pyrazoles III (R1 = CO2H, PhCHOH; resp.).
IT **71443-54-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and acidity of Me groups in)
RN 71443-54-4 CAPLUS
CN 1H-Pyrazole, 1,5-dimethyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)

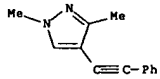


IT **71443-55-5P 71443-56-6P 71443-57-7P 71443-58-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 71443-55-5 CAPLUS
CN 1H-Pyrazole, 1-methyl-5-(methyl-d)-4-(phenylethynyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 47 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1978:62331 CAPLUS
DOCUMENT NUMBER: 88:62331
TITLE: New rearrangement of chloroethynylpyrazoles
AUTHOR(S): Sinyakov, A. N.; Vasilevskii, S. F.; Shvartsberg, M. S.
CORPORATE SOURCE: Inst. Khim. Kinet. Goreniya, Novosibirsk, USSR
SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1977), (10), 2306-10
CODEN: IASKA6; ISSN: 0002-3353
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 88:62331
GI

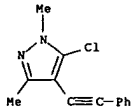


AB Treatment of pyrazole I (R = C.tplbond.CCl, R1 = H) (II) with NaNH2-NH3(l) gave 80% I (R = C.tplbond.CH, R1 = Cl) and 10% I (R = C.tplbond.CH, R1 = H). Rearrangement of II in the presence of I (R = C.tplbond.CPh, R1 = H) gave 70% I (R = C.tplbond.CH, R1 = Cl) and 14.3% I (R = C.tplbond.CPh, R1 = Cl). Analogously, pyrazoles III [R = 3(or5)-C.tplbond.CH] chlorinated with KClO gave III [R = 3(or 5)-C.tplbond.CCl] which were rearranged to give IV and ethynylmethylpyrazoles.
IT **65447-56-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with chloroethynylpyrazole)
RN 65447-56-5 CAPLUS
CN 1H-Pyrazole, 1,3-dimethyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)



IT **65447-57-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 65447-57-6 CAPLUS
CN 1H-Pyrazole, 5-chloro-1,3-dimethyl-4-(phenylethynyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 47 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L4 ANSWER 48 OF 48 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1971:463684 CAPLUS
DOCUMENT NUMBER: 75:63684
TITLE: Cycloaddition of diazomethane to conjugated diynes
AUTHOR(S): Stephan, Elie; Vo-Quang, Liliane; Vo-Quang-Yen
CORPORATE SOURCE: Lab. Rech. Chem. Org., Ec. Natl. Super. Chim. Paris, Paris, Fr.
SOURCE: Comptes Rendus des Seances de l'Academie des Sciences, Serie C: Sciences Chimiques (1971), 272(20), 1731-3
CODEN: CHDCAQ; ISSN: 0567-6541
DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 75:63684

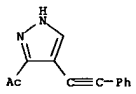
GI For diagram(s), see printed CA Issue.

AB Diazomethane adds exclusively to the α,β-triple bond of diynes ArC.tplbond.CC.tplbond.COR. Thus, the diynes are treated with CH_2N_2 to give pyrazoles (I) , (II), (III), and (IV) (R1 = H). I (R1 = H) and II (R1 = H) are the major products. I, II, III, and IV (Ar = Ph, p-tolyl, p-BrC6H4, p-ClC6H4; R = Me, Ph, OMe) are prepared, and NMR spectral data are given.

IT **33162-55-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 33162-55-9 CAPLUS

CN Ketone, methyl 4-(phenylethynyl)pyrazol-3-yl (8CI) (CA INDEX NAME)



=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	237.57	399.11

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-35.04	-35.04

STN INTERNATIONAL LOGOFF AT 14:55:53 ON 17 FEB 2005